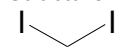


Name: Methylene Iodide
IUPAC-Name: Diiodomethane

Sum formula: CH₂I₂
CAS-Ref.-No.: 75-11-6
Structure formula:



Beilstein-Ref.: E IV 1, p. 96
Merck-Index: 11,5985; 12,6143
Smiles Notation: C(I)I

Synonyms: Methylene diiodide; Dijodmethan; Methylenjodid; Mi-gee; Methyl diiodide

Property	Coeffic./Unit	Value	Notes/References
Molecular Weight	g/mol	267.836	based on IUPAC 1995 Atomic Weights: T.B. Coplen, J. Phys. Chem. Ref. Data 26 (1997), p. 1239
Critical Temperature	K	747.87	estim. rev. Lydersen method
		740.92	estim. Joback method
Critical Pressure	bar	47.32	estim. rev. Lydersen method
		54.23	estim. Joback method
Critical Volume	cm ³ /mol	252.3	estim. rev. Lydersen method
		267.5	estim. Joback method
Melting Point	K	279.25	CRC Hdb 97/98 #7506 [1]
	°C	6.1	CRC Hdb 97/98 #7506 [1]
Normal Boiling Point	K	455.2	CRC Hdb 97/98 #7506 [1]
	°C	182	CRC Hdb 97/98 #7506 [1]
Density	g/cm ³	3.3254	@ 293 K, D'Ans-Lax, 1998, p.1017
		3.3212	@ 20 °C, CRC Hdb 97/98 #7506 [1]
		3.3079	@ 25 °C, Riddick et al. 1986 [5]
Density Function d = Density (g/cm ³)	A, g/cm ³	3.3707 ± 0.0019	d = A + BT + BT ² , T = temperature (°C) eval. regression with meas. data from A.I. Vogel et. al., J. Chem. Soc. 1948, p. 1850, V. Griffing et al., J. Phys. Chem. 58 (1954) p. 1054, Beilstein E III 1, p. 100
Tmin (12 °C)	B, g/cm ³ /K	-2.4958E-3	@ 20 °C, eval. from Density, CRC Hdb 97/98 #7506
Tmax (120 °C)	C, g/cm ³ /K ²	-8.6689E-8	
Molar Volume	cm ³ /mol	80.64	@ 20 °C, eval. from Density, CRC Hdb 97/98 #7506
Color/Odor	-	-	Light-yellow, clear liquid with a chloroform like odor, light-sensitive
Flash Point	°C	>112	Catalog Acros Organics
Vapor Pressure @ 20 °C	Torr	0.85	Riddick et al. 1986 [5]
Vapor Pressure Equation Parameters			from Vapor Pressure Equation Parameters
P = Vapor pressure (bar)	A	39.5746	log ₁₀ (P) = A + BT + C log ₁₀ (T) + DT ² , T = temp. (K) eval. Daubert et al., 1989 [6]
Tmin (279.25 K)	B, 1/K	-4052.75	eval. Daubert et al., 1989 [6]
Tmax (747.00 K)	C	-11.711	eval. Daubert et al., 1989 [6]
Acentric Factor	1	0.1468	eval. Daubert et al., 1989 [6]
		0.1405	eval. Lee-Kessler Equation Parameters eval. Daubert et al., 1989 [6], T _c = 747.00 K
IG Enthalpy of Formation kJ/mol		118.0 ± 4.2	meas. Kudchadker and Kudchadker, 1976 [8]
		90.0	estim. MOPAC 6.0, MNDO method (21.50 kcal/mol)
		90.0	estim. MOPAC 6.0, AM1 method (21.50 kcal/mol)
		89.8	estim. Joback method (21.44 kcal/mol)
Liq Enthalpy of Formation	kJ/mol	68.5 ± 0.8	meas. Carson, Laye, et al., 1993 [10]
Enthalpy of Fusion	kJ/mol	12.05	@ 279.25 K, Daubert et al., 1989 [6]
Enthalpy of Vaporization	kJ/mol	45.6	@ 298.15 K, meas. Carson, Laye, et al., 1994 [13]
		43.09	@ 298.15 K, estim. Watson method
		44.20	@ 298.15 K, estim. Pitzer method
		49.36	@ 298.15 K, eval. Daubert et al., 1989 [6]
Index of Refraction n _{D,20}	-	1.7425	@ 20 °C, CRC Hdb 97/98 #7506 [1]
		1.74108	@ 20 °C, A.I. Vogel et. al., J. Chem. Soc. 1948, p. 1850
Molar Refraction: R _{D,20}	cm ³	32.57	@ 20 °C, eval. from n _{D,20} , CRC Hdb 97/98 #7506 [1]
Polarizability	Å ³	12.90	CRC Hdb 97/98, p. 10-206
		13.00	estim. MOPAC 6.0, MNDO method
		12.42	estim. Group contributions method
Ionization Energy	eV	9.46 ± 0.02	meas. Tsai, Baer, et al., 1975 [14]
		10.87	estim. Hyperchem 5.02, MNDO method
		10.56	estim. Hyperchem 5.02, AM1 method

Property	Coeffic./Unit	Value	Notes/References
Constant Pressure Heat Capacity of liquid	J/(mol K)	133.81	@ 298.15 K, meas. Carson, Laye, et al., 1993 [10]
		112.8	@ 298.15 K, meas. Shehatta, 1993 [11]
		133.9	@ 298 K, meas. Kurbatov, 1948 [12]
Thermal Conductivity	W/(m K)	0.1015	@ 279.25 K, eval. Daubert et al., 1989 [6]
Viscosity	mPas	2.76 ± 0.05	@ 20 °C, eval. from regression, Yaws, 1995 [7]
Viscosity Function			$\log_{10}(\eta) = A + B/T + CT + DT^2$, T = temperature (K)
η = Dynamic Viscosity (mPas)	A, 1	-1.461	Yaws, 1995 [7]
Tmin (279 K)	B, K	507.43	
Tmax (747 K)	C, 1/K	0.0011256	
	D, 1/K ²	-1.847E-6	
Dielectric Constant (Permittivity)	1	5.32	@ 298.2 K, CRC Hdb 97/98, p. 6-141
		5.316	@ 25 °C, Riddick et al. 1986 [5]
Relative Permittivity Function			$\epsilon = A + BT + CT^2 + DT^3$, T = temperature (°C)
ϵ = Permittivity (1)	A, 1	-	
Tmin (°C)	B, 1/K	-	
Tmax (°C)	C, 1/K ²	-	
	D, 1/K ³	-	
Dipole Momentum:	D	1.08	@ 10..70 °C, meas. in Benzene, D'Ans-Lax [4], p. 3-303
		1.14	meas. in Hexane, Beilstein E III 1, p. 100
		1.10	meas. in Benzene, Beilstein E III 1, p. 100
		1.16	estim. Hyperchem 5.02, MNDO method
		1.13	estim. Hyperchem 5.02, AM1 method
Surface Tension	mN/m	50.88	@ 20 °C, G. Körösi et al., J. Chem. Eng. Data 26 (1981) p. 323
		50.0	H.J. Busscher et al., Coll. Surf. 9 (1984), p. 319-331
		50.8	F.M. Fowkes, Ind. Eng. Chem. 56 (1964) p. 48
		50.8	D.K.Owens et al., J. Appl. Polym. Sci. 13 (1969), p.1741
		50.8	G. Ström et al., J. Colloid Interf. Sci. 119 (1987), p. 352
Surface Tension Function			$\gamma = A + BT + CT^2$, T = temperature (°C)
γ = Surface Tension (mN/m)	A, mN/m	53.48 ± 0.07	from regression, LB IV/16, 1961-98 [3], p. 144
Tmin (0 °C)	B, mN/m/K	-0.14154	
Tmax (100 °C)	C, mN/m/K ²	4.9567E-5	
Dispersion Force Contribution of Surface Tension @ 20 °C	mN/m	47.4	H.J. Busscher et al, Coll. Surf. 9 (1984), p. 319-331
		48.5 ± 9	F.M. Fowkes, Ind. Eng. Chem. 56 (1964) p. 48
		49.5 ± 1	D.K.Owens et al., J. Appl. Polym. Sci. 13 (1969), p.1741
		50.8	G. Ström et al., J. Colloid Interf. Sci. 119 (1987), p. 352
		50.8	H.J. Busscher et al, Coll. Surf. 9 (1984), p. 319-331
Polar Force Contribution of Surface Tension @ 20 °C	mN/m	2.6	F.M. Fowkes, Ind. Eng. Chem. 56 (1964) p. 48
		2.3	D.K.Owens et al., J. Appl. Polym. Sci. 13 (1969), p.1741
		1.3	G. Ström et al., J. Colloid Interf. Sci. 119 (1987), p. 352
		0.0	M.L. Gonzalez-Martin et al., Langmuir 13 (1997), p. 5991
Acid-Base (A-B) Contributions of Surface Tension	total, mN/m	50.8	
	LW, mN/m	50.8	
	A, mN/m	0.72	
	B, mN/m	0.00	
Parachor	1	215.0	eval. from meas. Surface Tension and Density, CRC Hdb 97/98 #7506 [1]
Interfacial Tension vs. water	mN/m	35.86 ± 0.37	@ 20 °C, DataPhysics Instruments GmbH, 1998
		41.6	W. Fox: J. Am. Chem. Soc. 67 (1945) p. 700, E.G. Carter, D.C. Jones, Trans. Faraday Soc. 30 (1934) p. 1027
		48.50	@ 20 °C, W.D. Harkins, A. Feldmann, J. Am. Chem. Soc. 44 (1922) 2665 (2673)
Interfacial Tension vs. water Function			$\gamma_{ow} = A + BT$, T = temperature (°C)
γ_{ow} = Interfacial Tension (mN/m)	A, mN/m	38.04 ± 0.37	DataPhysics Instruments GmbH, 1998
Tmin (10 °C), Tmax (30 °C)	B, mN/m/K	-0.1085 ± 0.018	DataPhysics Instruments GmbH, 1998
Solubility in water	Mass-%	0.124	@ 30 °C, CRC Hdb 97/98, p. 8-87
Solubility of water	Mass-%	-	
Henry' Law Constant (water)	mol/kg bar	2.3	@ 298.15 K, Moore, Geen, et al., 1995 [19]
		2.8	@ 298.15 K, Yaws and Yang, 1992 [20]
		0.032	@ 25 °C, CRC Hdb 97/98, p. 8-87 [1]
$d(\ln(k^{\circ}_H))/d(1/T)$	K	5000	@ 298.15 K, Moore, Geen, et al., 1995 [19]

Property	Coeffic./Unit	Value	Notes/References
log P		2.30	meas. Pomona, 1987
		2.35	estim. LOGKOW, http://esc.syrres.com/~esc1/kowint.htm
		2.31	estim. Molecular Modeling Pro 3.0, group contrib.
		2.31	estim. CLOGP, http://www.daylight.com/daycgi/clogp
Hansen's 3D-Solubility Parameter			
total, @ 25 °C	MPa ^{1/2}	19.0	CRC Hdb SCS, 1997, p. 331 [17]
dispersion	MPa ^{1/2}	17.8	CRC Hdb SCS, 1997, p. 331 [17]
polar	MPa ^{1/2}	3.9	CRC Hdb SCS, 1997, p. 331 [17]
H-bonding	MPa ^{1/2}	5.5	CRC Hdb SCS, 1997, p. 331 [17]
Van der Waals Volume	cm ³ /mol	50.82 50.93	estim. Molecular Modeling Pro 3.0, MM2 geometry Daubert et al. 1989 [6]
Van der Waals Area	10 ⁹ cm ² /mol	6.832 6.430	estim. Molecular Modeling Pro 3.0, MM2 geometry Daubert et al. 1989 [6]

Structure

Molecular Structure (theor. calc., Hyperchem 5.02, AM1 method)

content of matrix:

column 1: element abbreviation, column 2: bond length in Å, column 3: vary? Y=1/N=0, column 4: bond angle in °,
column 5: vary? Y=1/N=0, column 6: dihedral angle in °, column 6: vary? Y=1/N=0, column 7: bond with atom #,
column 8: bond angle with atom # in column 7 and 8, column 9: dihedral angle with atom # in column 7, 8, and 9

AM1 UHF PRECISE GNORM=0.03

Name: D:\MOPAC6.0\Diiodmethane.mop

Sum formula: CH2I2

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C      00000.0000 0 00000.0000 0 00000.0000 0 0 0 0
H      00001.1077 1 00000.0000 0 00000.0000 0 1 0 0
H      00001.1077 1 00109.3146 1 00000.0000 0 1 2 0
I      00002.0418 1 00108.7105 1 00241.4761 1 1 2 3
I      00002.0417 1 00108.7161 1 00118.5339 1 1 2 3
0

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