BROMODICHLOROMETHANE

Other names:	BDCM
	CHBrCl2
	Dichlorobromomethane
	Dichloromonobromomethane
	Monobromodichloromethane
	NCI-C55243
	NSC 8018
	REFRIGERANT-20B1
	bromo-dichloromethane
	methane, bromodichloro-
Inchi:	InChI=1S/CHBrCl2/c2-1(3)4/h1H
InchiKey:	FMWLUWPQPKEARP-UHFFFAOYSA-N
Formula:	CHBrCl2
SMILES:	ClC(Cl)Br
Mol. weight [g/mol]:	163.83
CAS:	75-27-4

Physical Properties

Property code	Value	Unit	Source
af	0.2891		Cheméo Relay (1.0)
gf	-54.44	kJ/mol	Joback Method
hf	-48.36	kJ/mol	Cheméo Relay (1.0)
hfus	8.50	kJ/mol	Joback Method
hvap	36.22	kJ/mol	Cheméo Relay (1.0)
ie	10.96	eV	NIST Webbook
ie	10.88 ± 0.05	eV	NIST Webbook
ie	10.60	eV	NIST Webbook
log10ws	-1.54		Estimated Solubility Method
log10ws	-1.54		Aqueous Solubility Prediction Method
logp	2.143		Crippen Method
mcvol	66.930	ml/mol	McGowan Method
pc	5818.28	kPa	Joback Method
rinpol	690.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	706.00		NIST Webbook

rinpol	709.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	699.00		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	697.00		NIST Webbook
ripol	1175.89		NIST Webbook
ripol	1174.00		NIST Webbook
ripol	1167.37		NIST Webbook
ripol	1132.00		NIST Webbook
ripol	1132.00		NIST Webbook
ripol	1165.00		NIST Webbook
ripol	1132.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1174.75		NIST Webbook
tb	363.40 ± 0.50	K	NIST Webbook
tb	363.30 ± 0.50	K	NIST Webbook
tb	363.30 ± 0.60	K	NIST Webbook
tb	363.40 ± 0.50	K	NIST Webbook
tb	363.30 ± 0.50	K	NIST Webbook
tb	363.25	K	KDB
tb	362.50 ± 0.50	K	NIST Webbook
tb	361.60 ± 0.10	K	NIST Webbook
tc	573.88	K	Cheméo Relay (1.0)
tf	216.82	K	Aqueous Solubility Prediction Method
tf	216.00	K	NIST Webbook
tf	217.20 ± 0.40	K	NIST Webbook
vc	0.262	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	74.33	J/mol×K	362.86	Joback Method
cpg	85.96	J/mol×K	575.64	Joback Method
cpg	84.45	J/mol×K	540.18	Joback Method
cpg	82.79	J/mol×K	504.72	Joback Method
cpg	80.96	J/mol×K	469.25	Joback Method
cpg	78.95	J/mol×K	433.79	Joback Method
cpg	76.75	J/mol×K	398.32	Joback Method
dvisc	0.0010932	Pa×s	284.26	Joback Method
dvisc	0.0004838	Pa×s	362.86	Joback Method
dvisc	0.0006086	Pa×s	336.66	Joback Method
dvisc	0.0007957	Pa×s	310.46	Joback Method
dvisc	0.0046058	Pa×s	205.67	Joback Method
dvisc	0.0016019	Pa×s	258.07	Joback Method
dvisc	0.0025589	Pa×s	231.87	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52707e+01
Coeff. B	-3.86682e+03
Temperature range (K), min.	258.08
Temperature range (K), max.	388.47

Sources

Determination of Henry's Law Constants Using Internal Standards with Benchmark Values: https://www.doi.org/10.1021/je3010535

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C75274&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1516.mol
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume