CHLORODIBROMOMETHANE

Other names:	CDBM
	CHClBr2
	Chlorobromoform
	Chlorodibromethane
	Dibromomonochloromethane
	Methane, chlorodibromo-
	Monochlorodibromomethane
	NCI-C55254
	dibromo-chloromethane
	dibromochloromethane
Inchi:	InChI=1S/CHBr2Cl/c2-1(3)4/h1H
InchiKey:	GATVIKZLVQHOMN-UHFFFAOYSA-N
Formula:	CHBr2Cl
SMILES:	ClC(Br)Br
Mol. weight [g/mol]:	208.28

Physical Properties

Property code	Value	Unit	Source
af	0.3850		Cheméo Relay (1.0)
gf	-28.19	kJ/mol	Joback Method
hf	-7.77	kJ/mol	Cheméo Relay (1.0)
hfus	9.59	kJ/mol	Joback Method
hvap	40.88	kJ/mol	Cheméo Relay (1.0)
ie	10.59 ± 0.01	eV	NIST Webbook
ie	10.69	eV	NIST Webbook
ie	10.59 ± 0.01	eV	NIST Webbook
ie	10.50	eV	NIST Webbook
log10ws	-1.90		Aqueous Solubility Prediction Method
log10ws	-1.90		Estimated Solubility Method
logp	2.299		Crippen Method
mcvol	72.190	ml/mol	McGowan Method
pc	6886.93	kPa	Joback Method
rinpol	809.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	792.00		NIST Webbook

rinpol	775.00		NIST Webbook
rinpol	766.50		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	759.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	768.00		NIST Webbook
ripol	1310.00		NIST Webbook
ripol	1316.36		NIST Webbook
ripol	1322.01		NIST Webbook
ripol	1304.75		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1310.00		NIST Webbook
tb	384.37	K	Cheméo Relay (1.0)
tc	604.17	K	Cheméo Relay (1.0)
tf	251.82	K	Aqueous Solubility Prediction Method
vc	0.287	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	77.59	J/mol×K	391.59	Joback Method
cpg	88.75	J/mol×K	618.86	Joback Method
cpg	87.42	J/mol×K	580.98	Joback Method
cpg	85.91	J/mol×K	543.10	Joback Method
cpg	84.20	J/mol×K	505.22	Joback Method
cpg	82.26	J/mol×K	467.35	Joback Method

cpg	80.06	J/mol×K	429.47	Joback Method
dvisc	0.0011222	Pa×s	313.57	Joback Method
dvisc	0.0005291	Pa×s	391.59	Joback Method
dvisc	0.0006560	Pa×s	365.58	Joback Method
dvisc	0.0008405	Pa×s	339.58	Joback Method
dvisc	0.0039165	Pa×s	235.55	Joback Method
dvisc	0.0015786	Pa×s	287.56	Joback Method
dvisc	0.0023767	Pa×s	261.56	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C124481&Units=SI

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

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

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

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

Cheméo Relay (1.0):

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
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