Propane, 1,2-dibromo-3-chloro-

Other names:	1,2-Dibrom-3-chlor-propan
	1,2-Dibromo-3-Chloropropane
	1,2-Dibromo-3-cloro-propano
	1,2-Dibroom-3-chloorpropaan
	1,2-dibromo-3-chloropropane (DBCP)
	1-Chloro-2,3-dibromopropane
	3-Chloro-1,2-dibromopropane
	BBC 12
	ClCH2CHBrCH2Br
	DBCP
	Dibromchlorpropan
	Dibromochloropropane
	Fumagon
	Fumazone
	Fumazone 86
	Fumazone 86E
	NCI-C00500
	NSC 1512
	Nemabrom
	Nemafume
	Nemagon
	Nemagon 20
	Nemagon 20G
	Nemagon 90
	Nemagon Soil Fumigant
	Nemanax
	Nemapaz
	Nemaset
	Nemazon
	OS 1897
	Propane, 1-chloro-2,3-dibromo-
	SD 1897
Inchi:	InChI=1S/C3H5Br2Cl/c4-1-3(5)2-6/h3H,1-2H2
InchiKey:	WBEJYOJJBDISQU-UHFFFAOYSA-N
Formula:	C3H5Br2Cl
SMILES:	ClCC(Br)CBr
Mol. weight [g/mol]:	236.33
CAS:	96-12-8

Physical Properties

Property code	Value	Unit	Source
gf	-11.35	kJ/mol	Joback Method
hf	-73.61	kJ/mol	Joback Method
hfus	14.77	kJ/mol	Joback Method
hvap	39.14	kJ/mol	Joback Method
log10ws	-2.38		Aqueous Solubility Prediction Method
logp	2.384		Crippen Method
mcvol	100.370	ml/mol	McGowan Method
pc	5123.98	kPa	Joback Method
rinpol	1095.64		NIST Webbook
rinpol	1033.90		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1100.14		NIST Webbook
rinpol	1089.72		NIST Webbook
rinpol	1092.41		NIST Webbook
rinpol	1063.00		NIST Webbook
ripol	1657.00		NIST Webbook
tb	437.35	K	Joback Method
tc	658.89	K	Joback Method
tf	258.09	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	143.00	J/mol×K	437.35	Joback Method
cpg	148.99	J/mol×K	474.27	Joback Method
cpg	154.54	J/mol×K	511.20	Joback Method
cpg	159.68	J/mol×K	548.12	Joback Method
cpg	164.44	J/mol×K	585.04	Joback Method
cpg	168.85	J/mol×K	621.97	Joback Method
cpg	172.94	J/mol×K	658.89	Joback Method
dvisc	0.0039928	Pa×s	258.09	Joback Method
dvisc	0.0023005	Pa×s	287.97	Joback Method
dvisc	0.0014702	Pa×s	317.84	Joback Method
dvisc	0.0010147	Pa×s	347.72	Joback Method

dvisc	0.0007427	Pa×s	377.60	Joback Method
dvisc	0.0005690	Pa×s	407.47	Joback Method
dvisc	0.0004521	Pa×s	437.35	Joback Method

Sources

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96128&Units=SI

Legend

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
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