1,3-Propanediol, 2,2-bis(bromomethyl)-

Other names:	Dibromoneopentyl glycol
	Dibromopentaerythritol
	Pentaerythritol dibromide
	Pentaerythritol dibromohydrin
	1,3-Dibromo-2,2-dimethylolpropane
	2,2-Bis(bromomethyl)-1,3-propanediol
	2,2-Dibromomethyl-1,3-propanediol
	FR 1138
	NCI-C55516
	1,3-Propanediol, 2,2-bis(2-bromomethyl)-
	2,2-Bis(2-bromomethyl)-1,3-propanediol
	1,3-Dibromo-2,2-dihydroxymethylpropane
	FR 522
	DBNPG
	NSC 9001
	2,2-bis(bromomethyl)propane-1,3-diol
Inchi:	InChI=1S/C5H10Br2O2/c6-1-5(2-7,3-8)4-9/h8-9H,1-4H2
InchiKey:	CHUGKEQJSLOLHL-UHFFFAOYSA-N
Formula:	C5H10Br2O2
SMILES:	OCC(CO)(CBr)CBr
Mol. weight [g/mol]:	261.94
CAS:	3296-90-0

Physical Properties

Property code	Value	Unit	Source
gf	-250.94	kJ/mol	Joback Method
hf	-407.08	kJ/mol	Joback Method
hfus	20.04	kJ/mol	Joback Method
hvap	71.66	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.747		Crippen Method
mcvol	128.050	ml/mol	McGowan Method
pc	5430.51	kPa	Joback Method
tb	627.25	K	Joback Method
tc	818.86	K	Joback Method
tf	389.77	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.63	J/mol×K	627.25	Joback Method
cpg	283.17	J/mol×K	659.19	Joback Method
cpg	289.29	J/mol×K	691.12	Joback Method
cpg	295.01	J/mol×K	723.06	Joback Method
cpg	300.38	J/mol×K	754.99	Joback Method
cpg	305.44	J/mol×K	786.93	Joback Method
cpg	310.22	J/mol×K	818.86	Joback Method
dvisc	0.0044873	Pa×s	389.77	Joback Method
dvisc	0.0013654	Pa×s	429.35	Joback Method
dvisc	0.0005079	Pa×s	468.93	Joback Method
dvisc	0.0002204	Pa×s	508.51	Joback Method
dvisc	0.0001079	Pa×s	548.09	Joback Method
dvisc	0.0000581	Pa×s	587.67	Joback Method
dvisc	0.0000339	Pa×s	627.25	Joback Method
hfust	30.10	kJ/mol	387.30	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3296900&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

hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume