dl-2,3-Dibromo-1,4-butanediol

Other names:	1,4-Butanediol, 2,3-dibromo-, (R*,R*)-(.+/-.)- 1,4-BUTANEDIOL, 2,3-DIBROMO-, (+,-)- 1,4-Butanediol, d,l-2,3-dibromo- .+/-.-2,3-Dibromo-1,4-butanediol (R*,R*)-(±)-2,3-dibromobutane-1,4-diol
Inchi:	InChI=1S/C4H8Br2O2/c5-3(1-7)4(6)2-8/h3-4,7-8H,1-2H2
InchiKey:	OXYNQEOLHRWEPE-UHFFFAOYSA-N
Formula:	C4H8Br2O2
SMILES:	OCC(Br)C(Br)CO
Mol. weight [g/mol]:	247.91
CAS:	1947-58-6

Physical Properties

Property code	Value	Unit	Source
gf	-267.08	kJ/mol	Joback Method
hf	-388.25	kJ/mol	Joback Method
hfus	17.82	kJ/mol	Joback Method
hvap	69.95	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	0.498		Crippen Method
mcvol	113.960	ml/mol	McGowan Method
pc	6259.01	kPa	Joback Method
tb	606.72	K	Joback Method
tc	797.70	K	Joback Method
tf	346.08	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.20	J/mol×K	797.70	Joback Method
cpg	229.35	J/mol×K	606.72	Joback Method
cpg	235.10	J/mol×K	638.55	Joback Method
cpg	240.50	J/mol×K	670.38	Joback Method

cpg	245.59	J/mol×K	702.21	Joback Method
cpg	250.39	J/mol×K	734.04	Joback Method
cpg	254.91	J/mol×K	765.87	Joback Method
dvisc	0.0000437	Pa×s	606.72	Joback Method
dvisc	0.0163136	Pa×s	346.08	Joback Method
dvisc	0.0035058	Pa×s	389.52	Joback Method
dvisc	0.0010257	Pa×s	432.96	Joback Method
dvisc	0.0003755	Pa×s	476.40	Joback Method
dvisc	0.0001626	Pa×s	519.84	Joback Method
dvisc	0.0000801	Pa×s	563.28	Joback Method
hfust	29.29	kJ/mol	363.20	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	422.20	K	0.10	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=C1947586&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume