1,4-Dibromo-2-butanol

Other names: 2-Butanol, 1,4-dibromo-
1,4-Dibromobutan-2-ol
Inchi: InChI=1S/C4H8Br2O/c5-2-1-4(7)3-6/h4,7H,1-3H2
InchiKey: PSSRAPMBSMSACN-UHFFFAOYSA-N
Formula: C4H8Br2O
SMILES: OC(CBr)CCBr
Mol. weight [g/mol]: 231.91
CAS: 19398-47-1

Physical Properties

Property code	Value	Unit	Source
gf	-127.82	kJ/mol	Joback Method
hf	-230.74	kJ/mol	Joback Method
hfus	17.25	kJ/mol	Joback Method
hvap	53.66	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.527		Crippen Method
mcvol	108.090	ml/mol	McGowan Method
pc	5374.91	kPa	Joback Method
tb	514.98	K	Joback Method
tc	713.75	K	Joback Method
tf	300.26	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.16	J/mol×K	514.98	Joback Method
cpg	224.04	J/mol×K	680.62	Joback Method
cpg	218.77	J/mol×K	647.50	Joback Method
cpg	213.17	J/mol×K	614.37	Joback Method
cpg	207.22	J/mol×K	581.24	Joback Method
cpg	200.89	J/mol×K	548.11	Joback Method
cpg	229.01	J/mol×K	713.75	Joback Method

dvisc	0.0002148	Pa×s	514.98	Joback Method
dvisc	0.0003325	Pa×s	479.19	Joback Method
dvisc	0.0005525	Pa×s	443.41	Joback Method
dvisc	0.0010034	Pa×s	407.62	Joback Method
dvisc	0.0020443	Pa×s	371.83	Joback Method
dvisc	0.0048466	Pa×s	336.05	Joback Method
dvisc	0.0141153	Pa×s	300.26	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.70	K	1.70	NIST Webbook
tbrp	429.50 ± 3.50	K	6.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19398471&Units=SI
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

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
tb: Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume