

2,3-Dibromopropyl alcohol

Other names:	1-Propanol, 2,3-dibromo- 1,2-Dibromopropan-3-ol 2,3-Dibromo-1-propanol 2,3-Dibromopropanol 1,2-Dibromohydrin Brominex 257 NCI-C55436 USAF DO-42 DBP «beta»-Dibromohydrin DBP (flame retardant) NSC 6203 2,3-dibromopropan-1-ol
Inchi:	InChI=1S/C3H6Br2O/c4-1-3(5)2-6/h3,6H,1-2H2
InchiKey:	QWVCIORZLNBIIC-UHFFFAOYSA-N
Formula:	C3H6Br2O
SMILES:	OCC(Br)CBr
Mol. weight [g/mol]:	217.89
CAS:	96-13-9

Physical Properties

Property code	Value	Unit	Source
gf	-136.24	kJ/mol	Joback Method
hf	-210.10	kJ/mol	Joback Method
hfus	14.66	kJ/mol	Joback Method
hvap	51.43	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.137		Crippen Method
mcvol	94.000	ml/mol	McGowan Method
pc	6219.59	kPa	Joback Method
rinpol	1079.00		NIST Webbook
rinpol	1079.00		NIST Webbook
tb	492.10	K	Joback Method
tc	693.60	K	Joback Method
tf	288.99	K	Joback Method
vc	0.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.18	J/molxK	492.10	Joback Method
cpg	160.65	J/molxK	525.68	Joback Method
cpg	165.78	J/molxK	559.27	Joback Method
cpg	170.57	J/molxK	592.85	Joback Method
cpg	175.07	J/molxK	626.43	Joback Method
cpg	179.28	J/molxK	660.02	Joback Method
cpg	183.24	J/molxK	693.60	Joback Method
dvisc	0.0172793	Paxs	288.99	Joback Method
dvisc	0.0059899	Paxs	322.84	Joback Method
dvisc	0.0025389	Paxs	356.69	Joback Method
dvisc	0.0012488	Paxs	390.55	Joback Method
dvisc	0.0006879	Paxs	424.40	Joback Method
dvisc	0.0004138	Paxs	458.25	Joback Method
dvisc	0.0002669	Paxs	492.10	Joback Method
hvapt	57.30	kJ/mol	411.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.20	K	1.30	NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C96139&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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