

2-Propanol, 1,3-dibromo-

Other names:	«alpha»-Dibromohydrin «alpha»,«gamma»-Dibromohydrin Glycerol «alpha»,«gamma»-dibromohydrin Glycerol 1,3-dibromohydrin 1,3-Dibromo-2-hydroxypropane 1,3-Dibromo-2-propanol 1,3-Dibromohydrin Glycerol «alpha»,«gamma»-dibromohydrine 2-Hydroxy-1,3-dibromopropane 1,3-Dibromopropanol NSC 636 1,3-dibromopropan-2-ol
Inchi:	InChI=1S/C3H6Br2O/c4-1-3(6)2-5/h3,6H,1-2H2
InchiKey:	KIHQZLPHVZKELA-UHFFFAOYSA-N
Formula:	C3H6Br2O
SMILES:	OC(CBr)CBr
Mol. weight [g/mol]:	217.89
CAS:	96-21-9

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
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/mol×K	492.10	Joback Method
cpg	160.65	J/mol×K	525.68	Joback Method
cpg	165.78	J/mol×K	559.27	Joback Method
cpg	170.57	J/mol×K	592.85	Joback Method
cpg	175.07	J/mol×K	626.43	Joback Method
cpg	179.28	J/mol×K	660.02	Joback Method
cpg	183.24	J/mol×K	693.60	Joback Method
dvisc	0.0172793	Pa×s	288.99	Joback Method
dvisc	0.0059899	Pa×s	322.84	Joback Method
dvisc	0.0025389	Pa×s	356.69	Joback Method
dvisc	0.0012488	Pa×s	390.55	Joback Method
dvisc	0.0006879	Pa×s	424.40	Joback Method
dvisc	0.0004138	Pa×s	458.25	Joback Method
dvisc	0.0002669	Pa×s	492.10	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.70	K	0.90	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=C96219&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
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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