

2-Propanol, 1,3-bis(dimethylamino)-

Other names:	1,3-Bis(dimethylamino)-2-hydroxypropane 1,3-Bis(dimethylamino)-2-propanol 1,3-Bis(dimethylamino)isopropanol 1,3-bis(dimethylamino)propan-2-ol
Inchi:	InChI=1S/C7H18N2O/c1-8(2)5-7(10)6-9(3)4/h7,10H,5-6H2,1-4H3
InchiKey:	JGVZJRHAZOBPMW-UHFFFAOYSA-N
Formula:	C7H18N2O
SMILES:	CN(C)CC(O)CN(C)C
Mol. weight [g/mol]:	146.23
CAS:	5966-51-8

Physical Properties

Property code	Value	Unit	Source
gf	90.36	kJ/mol	Joback Method
hf	-210.26	kJ/mol	Joback Method
hfus	20.49	kJ/mol	Joback Method
hvap	51.55	kJ/mol	Joback Method
log10ws	0.73		Crippen Method
logp	-0.529		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
tb	476.18	K	Joback Method
tc	637.36	K	Joback Method
tf	279.41	K	Joback Method
vc	0.476	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.49	J/molxK	476.18	Joback Method
cpg	324.01	J/molxK	503.04	Joback Method
cpg	335.98	J/molxK	529.91	Joback Method
cpg	347.41	J/molxK	556.77	Joback Method
cpg	358.34	J/molxK	583.63	Joback Method

cpg	368.77	J/mol×K	610.50	Joback Method
cpg	378.73	J/mol×K	637.36	Joback Method
hvapt	50.30	kJ/mol	402.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	354.00 ± 1.00	K	2.30	NIST Webbook

Sources

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=C5966518&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
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
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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