

3-Dipropylamino-1,2-propanediol

Other names:	1,2-Propanediol, 3-(dipropylamino)- 3-(dipropylamino)propane-1,2-diol
Inchi:	InChI=1S/C9H21NO2/c1-3-5-10(6-4-2)7-9(12)8-11/h9,11-12H,3-8H2,1-2H3
InchiKey:	CTSOJEIWXRSEM-UHFFFAOYSA-N
Formula:	C9H21NO2
SMILES:	CCCN(CCC)CC(O)CO
Mol. weight [g/mol]:	175.27
CAS:	60302-96-7

Physical Properties

Property code	Value	Unit	Source
gf	-140.40	kJ/mol	Joback Method
hf	-471.30	kJ/mol	Joback Method
hfus	26.74	kJ/mol	Joback Method
hvap	70.64	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	0.462		Crippen Method
mvol	159.390	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
tb	601.68	K	Joback Method
tc	760.27	K	Joback Method
tf	330.30	K	Joback Method
vc	0.590	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.31	J/molxK	601.68	Joback Method
cpg	440.93	J/molxK	628.11	Joback Method
cpg	452.05	J/molxK	654.54	Joback Method
cpg	462.69	J/molxK	680.98	Joback Method
cpg	472.87	J/molxK	707.41	Joback Method
cpg	482.60	J/molxK	733.84	Joback Method
cpg	491.91	J/molxK	760.27	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.20	K	1.00	NIST Webbook

Sources

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=C60302967&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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