

2-Dimethylamino-1-propanol

Other names:	2-(dimethylamino)propan-1-ol
Inchi:	InChI=1S/C5H13NO/c1-5(4-7)6(2)3/h5,7H,4H2,1-3H3
InchiKey:	PBKGYWLWIJLDGZ-UHFFFAOYSA-N
Formula:	C5H13NO
SMILES:	CC(CO)N(C)C
Mol. weight [g/mol]:	103.16
CAS:	15521-18-3

Physical Properties

Property code	Value	Unit	Source
gf	-37.26	kJ/mol	Joback Method
hf	-236.51	kJ/mol	Joback Method
hfus	12.29	kJ/mol	Joback Method
hvap	45.06	kJ/mol	Joback Method
log10ws	0.14		Crippen Method
logp	-0.071		Crippen Method
mcvol	97.160	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
tb	417.98	K	Joback Method
tc	581.92	K	Joback Method
tf	224.40	K	Joback Method
vc	0.346	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.91	J/mol×K	417.98	Joback Method
cpg	207.62	J/mol×K	445.30	Joback Method
cpg	216.93	J/mol×K	472.63	Joback Method
cpg	225.85	J/mol×K	499.95	Joback Method
cpg	234.40	J/mol×K	527.28	Joback Method
cpg	242.58	J/mol×K	554.60	Joback Method
cpg	250.40	J/mol×K	581.92	Joback Method

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=C15521183&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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