

Cyclohexanol, 3-(aminomethyl)-3,5,5-trimethyl-

Other names:	3-Aminomethyl-3,5,5-trimethylcyclohexanol 3-aminomethyl-3,5,5-trimethylcyclohexan-1-ol
Inchi:	InChI=1S/C10H21NO/c1-9(2)4-8(12)5-10(3,6-9)7-11/h8,12H,4-7,11H2,1-3H3
InchiKey:	YFEAYNIMJBHJCM-UHFFFAOYSA-N
Formula:	C10H21NO
SMILES:	CC1(C)CC(O)CC(C)(CN)C1
Mol. weight [g/mol]:	171.28
CAS:	15647-11-7

Physical Properties

Property code	Value	Unit	Source
gf	-39.00	kJ/mol	Joback Method
hf	-324.05	kJ/mol	Joback Method
hfus	12.32	kJ/mol	Joback Method
hvap	62.68	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.522		Crippen Method
mcvol	156.750	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
tb	538.20	K	NIST Webbook
tc	812.76	K	Joback Method
tf	393.24	K	Joback Method
vc	0.571	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.01	J/mol×K	603.60	Joback Method
cpg	451.16	J/mol×K	638.46	Joback Method
cpg	466.50	J/mol×K	673.32	Joback Method
cpg	481.22	J/mol×K	708.18	Joback Method
cpg	495.47	J/mol×K	743.04	Joback Method
cpg	509.43	J/mol×K	777.90	Joback Method
cpg	523.28	J/mol×K	812.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15647117&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvp:	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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