5-Amino-2,2-dimethylpentanol

Other names: 2,2-Dimethyl-5-amino-1-pentanol
Inchi: InChI=1S/C7H17NO/c1-7(2,6-9)4-3-5-8/h9H,3-6,8H2,1-2H3
InchiKey: ZOOPONUAQQEUQX-UHFFFAOYSA-N
Formula: C7H17NO
SMILES: CC(C)(CO)CCCN
Mol. weight [g/mol]: 131.22
CAS: 13532-77-9

Physical Properties

Property code	Value	Unit	Source
gf	-59.47	kJ/mol	Joback Method
hf	-315.00	kJ/mol	Joback Method
hfus	15.76	kJ/mol	Joback Method
hvap	57.20	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	0.744		Crippen Method
mcvol	125.340	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
tb	521.04	K	Joback Method
tc	702.26	K	Joback Method
tf	315.15	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.56	J/mol×K	521.04	Joback Method
cpg	319.23	J/mol×K	551.24	Joback Method
cpg	330.30	J/mol×K	581.45	Joback Method
cpg	340.80	J/mol×K	611.65	Joback Method
cpg	350.75	J/mol×K	641.85	Joback Method
cpg	360.18	J/mol×K	672.06	Joback Method
cpg	369.12	J/mol×K	702.26	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	499.00	K	98.00	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=C13532779&Units=SI

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