

N-2-(1-hydroxy-2-methyl) propylacetamide

Inchi: InChI=1S/C6H13NO2/c1-5(9)7-6(2,3)4-8/h8H,4H2,1-3H3,(H,7,9)
InchiKey: WSEURCHZECZCGQ-UHFFFAOYSA-N
Formula: C6H13NO2
SMILES: CC(O)=NC(C)(C)CO
Mol. weight [g/mol]: 131.17
CAS: 1569-96-6

Physical Properties

Property code	Value	Unit	Source
hf	-407.95	kJ/mol	Joback Method
hvac	64.41	kJ/mol	Joback Method
log10ws	-0.69		Crippen Method
logp	0.734		Crippen Method
mccvol	112.820	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
tb	594.37	K	Joback Method
tc	777.69	K	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=C1569966&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions
hvac: 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

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