N-2-(1,3-dihydroxy-2-methylpropyl) acetamide

Inchi: InChI=1S/C6H13NO3/c1-5(10)7-6(2,3-8)4-9/h8-9H,3-4H2,1-2H3,(H,7,10)
InchiKey: XFACEAHMBQFBTP-UHFFFAOYSA-N
Formula: C6H13NO3
SMILES: CC(=O)NC(C)(CO)CO
Mol. weight [g/mol]: 147.17
CAS: 66671-83-8

Physical Properties

Property code	Value	Unit	Source
gf	-310.69	kJ/mol	Joback Method
hf	-539.49	kJ/mol	Joback Method
hfus	18.76	kJ/mol	Joback Method
hvap	74.19	kJ/mol	Joback Method
log10ws	0.06		Crippen Method
logp	-1.134		Crippen Method
mcvol	118.690	ml/mol	McGowan Method
pc	4356.87	kPa	Joback Method
tb	621.85	K	Joback Method
tc	798.13	K	Joback Method
tf	384.03	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.33	J/mol×K	621.85	Joback Method
cpg	323.63	J/mol×K	651.23	Joback Method
cpg	331.48	J/mol×K	680.61	Joback Method
cpg	338.89	J/mol×K	709.99	Joback Method
cpg	345.88	J/mol×K	739.37	Joback Method
cpg	352.49	J/mol×K	768.75	Joback Method
cpg	358.73	J/mol×K	798.13	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=C66671838&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