N-1-(2-hydroxybutyl) acetamide

Inchi: InChI=1S/C6H13NO2/c1-3-6(9)4-7-5(2)8/h6,9H,3-4H2,1-2H3,(H,7,8)
InchiKey: LTKKVHOQYLMJFD-UHFFFAOYSA-N
Formula: C6H13NO2
SMILES: CCC(O)CNC(C)=O
Mol. weight [g/mol]: 131.17
CAS: 4293-58-7

Physical Properties

Property code	Value	Unit	Source
gf	-179.15	kJ/mol	Joback Method
hf	-383.79	kJ/mol	Joback Method
hfus	18.56	kJ/mol	Joback Method
hvap	58.42	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	-0.107		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
tb	532.46	K	Joback Method
tc	709.96	K	Joback Method
tf	305.79	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.57	J/mol×K	532.46	Joback Method
cpg	276.18	J/mol×K	562.04	Joback Method
cpg	285.37	J/mol×K	591.63	Joback Method
cpg	294.13	J/mol×K	621.21	Joback Method
cpg	302.48	J/mol×K	650.79	Joback Method
cpg	310.44	J/mol×K	680.38	Joback Method
cpg	318.01	J/mol×K	709.96	Joback Method

Sources

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=C4293587&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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