N-2-(1-acetoxy-3-methyl) butylacetamide

Inchi: InChI=1S/C9H17NO3/c1-6(2)9(10-7(3)11)5-13-8(4)12/h6,9H,5H2,1-4H3,(H,10,11)
InchiKey: GLDGDNNKPSKFAO-UHFFFAOYSA-N
Formula: C9H17NO3
SMILES: CC(=O)NC(COC(C)=O)C(C)C
Mol. weight [g/mol]: 187.24
CAS: 4146-09-2

Physical Properties

Property code	Value	Unit	Source
gf	-253.43	kJ/mol	Joback Method
hf	-543.56	kJ/mol	Joback Method
hfus	21.51	kJ/mol	Joback Method
hvap	57.19	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	0.710		Crippen Method
mcvol	156.660	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
tb	584.77	K	Joback Method
tc	776.33	K	Joback Method
tf	335.94	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.51	J/mol×K	584.77	Joback Method
cpg	406.78	J/mol×K	616.70	Joback Method
cpg	419.40	J/mol×K	648.62	Joback Method
cpg	431.40	J/mol×K	680.55	Joback Method
cpg	442.78	J/mol×K	712.47	Joback Method
cpg	453.53	J/mol×K	744.40	Joback Method
cpg	463.68	J/mol×K	776.33	Joback Method

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=C4146092&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume