N-(1,4-dimethylpentyl) acetoacetamide

Inchi: InChI=1S/C11H21NO2/c1-8(2)5-6-9(3)12-11(14)7-10(4)13/h8-9H,5-7H2,1-4H3,(H,12,14)
InchiKey: NDOJWLCHAUMMPF-UHFFFAOYSA-N
Formula: C11H21NO2
SMILES: CC(=O)CC(=O)NC(C)CCC(C)C
Mol. weight [g/mol]: 199.29
CAS: 73622-68-1

Physical Properties

Property code	Value	Unit	Source
gf	-131.59	kJ/mol	Joback Method
hf	-452.62	kJ/mol	Joback Method
hfus	25.50	kJ/mol	Joback Method
hvap	59.23	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	1.906		Crippen Method
mcvol	178.970	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
tb	608.11	K	Joback Method
tc	796.58	K	Joback Method
tf	336.25	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.32	J/mol×K	608.11	Joback Method
cpg	481.14	J/mol×K	639.52	Joback Method
cpg	495.21	J/mol×K	670.93	Joback Method
cpg	508.56	J/mol×K	702.35	Joback Method
cpg	521.20	J/mol×K	733.76	Joback Method
cpg	533.15	J/mol×K	765.17	Joback Method
cpg	544.43	J/mol×K	796.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73622681&Units=SI
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

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