2-Acetylamino-octanoic acid methyl ester

Inchi: InChI=1S/C11H21NO3/c1-4-5-6-7-8-10(11(14)15-3)12-9(2)13/h10H,4-8H2,1-3H3,(H,12,1
InchiKey: HXEHVYHMGGXHQE-UHFFFAOYSA-N
Formula: C11H21NO3
SMILES: CCCCCCC(NC(C)=O)C(=O)OC
Mol. weight [g/mol]: 215.29

Physical Properties

Property code	Value	Unit	Source
gf	-234.15	kJ/mol	Joback Method
hf	-579.56	kJ/mol	Joback Method
hfus	30.21	kJ/mol	Joback Method
hvap	62.03	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.635		Crippen Method
mcvol	184.840	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1539.00		NIST Webbook
rinpol	1539.00		NIST Webbook
tb	630.97	K	Joback Method
tc	815.25	K	Joback Method
tf	373.48	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.58	J/mol×K	630.97	Joback Method
cpg	506.86	J/mol×K	661.68	Joback Method
cpg	520.46	J/mol×K	692.40	Joback Method
cpg	533.37	J/mol×K	723.11	Joback Method
cpg	545.62	J/mol×K	753.82	Joback Method
cpg	557.21	J/mol×K	784.54	Joback Method
cpg	568.15	J/mol×K	815.25	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=R247691&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume