

Acetoxyacetamide, N,N-dihexyl-

Inchi:	InChI=1S/C16H31NO3/c1-4-6-8-10-12-17(13-11-9-7-5-2)16(19)14-20-15(3)18/h4-14H2,1
InchiKey:	IVLFEIWEQQLURU-UHFFFAOYSA-N
Formula:	C16H31NO3
SMILES:	CCCCCN(CCCCC)C(=O)COC(C)=O
Mol. weight [g/mol]:	285.42

Physical Properties

Property code	Value	Unit	Source
gf	-168.22	kJ/mol	Joback Method
hf	-663.42	kJ/mol	Joback Method
hfus	44.60	kJ/mol	Joback Method
hvap	69.16	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.539		Crippen Method
mvol	255.290	ml/mol	McGowan Method
pc	1427.22	kPa	Joback Method
rinpol	1994.00		NIST Webbook
rinpol	1994.00		NIST Webbook
tb	708.08	K	Joback Method
tc	883.14	K	Joback Method
tf	424.64	K	Joback Method
vc	0.980	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.72	J/molxK	708.08	Joback Method
cpg	761.70	J/molxK	737.26	Joback Method
cpg	777.84	J/molxK	766.43	Joback Method
cpg	793.16	J/molxK	795.61	Joback Method
cpg	807.68	J/molxK	824.79	Joback Method
cpg	821.43	J/molxK	853.96	Joback Method
cpg	834.42	J/molxK	883.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U308293&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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