Acetoxyacetamide, N,N-diheptyl-

Inchi: InChI=1S/C18H35NO3/c1-4-6-8-10-12-14-19(15-13-11-9-7-5-2)18(21)16-22-17(3)20/h4-1
InchiKey: PBWNUGZZRBCKFE-UHFFFAOYSA-N
Formula: C18H35NO3
SMILES: CCCCCCCN(CCCCCCC)C(=O)COC(C)=O
Mol. weight [g/mol]: 313.48

Physical Properties

Property code	Value	Unit	Source
gf	-151.38	kJ/mol	Joback Method
hf	-704.70	kJ/mol	Joback Method
hfus	49.78	kJ/mol	Joback Method
hvap	73.61	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.319		Crippen Method
mcvol	283.470	ml/mol	McGowan Method
pc	1240.71	kPa	Joback Method
rinpol	2185.00		NIST Webbook
rinpol	2185.00		NIST Webbook
tb	753.84	K	Joback Method
tc	931.11	K	Joback Method
tf	447.18	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.75	J/mol×K	753.84	Joback Method
cpg	878.53	J/mol×K	783.38	Joback Method
cpg	895.40	J/mol×K	812.93	Joback Method
cpg	911.37	J/mol×K	842.47	Joback Method
cpg	926.47	J/mol×K	872.02	Joback Method
cpg	940.74	J/mol×K	901.56	Joback Method
cpg	954.19	J/mol×K	931.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308296&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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