«beta»-Alanine, N-acryloyl-, dodecyl ester

Inchi: InChI=1S/C18H33NO3/c1-3-5-6-7-8-9-10-11-12-13-16-22-18(21)14-15-19-17(20)4-2/h4H
InchiKey: DRTDMOMXTHYZLJ-UHFFFAOYSA-N
Formula: C18H33NO3
SMILES: C=CC(=O)NCCC(=O)OCCCCCCCCCCCC
Mol. weight [g/mol]: 311.46

Physical Properties

Property code	Value	Unit	Source
gf	-84.93	kJ/mol	Joback Method
hf	-593.33	kJ/mol	Joback Method
hfus	50.58	kJ/mol	Joback Method
hvap	77.33	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.143		Crippen Method
mcvol	279.170	ml/mol	McGowan Method
pc	1292.07	kPa	Joback Method
rinpol	2409.00		NIST Webbook
tb	788.25	K	Joback Method
tc	971.95	K	Joback Method
tf	465.61	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.35	J/mol×K	788.25	Joback Method
cpg	872.04	J/mol×K	818.87	Joback Method
cpg	887.81	J/mol×K	849.48	Joback Method
cpg	902.69	J/mol×K	880.10	Joback Method
cpg	916.70	J/mol×K	910.72	Joback Method
cpg	929.88	J/mol×K	941.33	Joback Method
cpg	942.24	J/mol×K	971.95	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=U321682&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume