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

Inchi: InChI=1S/C14H25NO3/c1-3-5-6-7-8-9-12-18-14(17)10-11-15-13(16)4-2/h4H,2-3,5-12H2,
InchiKey: QYDKMEPMIQMPBO-UHFFFAOYSA-N
Formula: C14H25NO3
SMILES: C=CC(=O)NCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 255.35

Physical Properties

Property code	Value	Unit	Source
gf	-118.61	kJ/mol	Joback Method
hf	-510.77	kJ/mol	Joback Method
hfus	40.22	kJ/mol	Joback Method
hvap	68.43	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.582		Crippen Method
mcvol	222.810	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
rinpol	2002.00		NIST Webbook
rinpol	2002.00		NIST Webbook
tb	696.73	K	Joback Method
tc	877.76	K	Joback Method
tf	420.53	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.12	J/mol×K	696.73	Joback Method
cpg	643.14	J/mol×K	726.90	Joback Method
cpg	657.39	J/mol×K	757.07	Joback Method
cpg	670.90	J/mol×K	787.24	Joback Method
cpg	683.68	J/mol×K	817.41	Joback Method
cpg	695.75	J/mol×K	847.58	Joback Method
cpg	707.13	J/mol×K	877.76	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=U321680&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