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

Inchi: InChI=1S/C12H21NO3/c1-3-5-6-7-10-16-12(15)8-9-13-11(14)4-2/h4H,2-3,5-10H2,1H3,(H
InchiKey: GAYWMVGWTMPYMR-UHFFFAOYSA-N
Formula: C12H21NO3
SMILES: C=CC(=O)NCCC(=O)OCCCCCC
Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
gf	-135.45	kJ/mol	Joback Method
hf	-469.49	kJ/mol	Joback Method
hfus	35.04	kJ/mol	Joback Method
hvap	63.97	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	1.802		Crippen Method
mcvol	194.630	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	1787.00		NIST Webbook
tb	650.97	K	Joback Method
tc	833.66	K	Joback Method
tf	397.99	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.51	J/mol×K	650.97	Joback Method
cpg	535.54	J/mol×K	681.42	Joback Method
cpg	548.87	J/mol×K	711.87	Joback Method
cpg	561.51	J/mol×K	742.31	Joback Method
cpg	573.49	J/mol×K	772.76	Joback Method
cpg	584.82	J/mol×K	803.21	Joback Method
cpg	595.52	J/mol×K	833.66	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=U321679&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