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

Inchi: InChI=1S/C12H21NO3/c1-4-11(14)13-8-7-12(15)16-9-5-6-10(2)3/h4,10H,1,5-9H2,2-3H3,
InchiKey: LGODNLCNMQBMAP-UHFFFAOYSA-N
Formula: C12H21NO3
SMILES: C=CC(=O)NCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
gf	-137.89	kJ/mol	Joback Method
hf	-474.77	kJ/mol	Joback Method
hfus	31.52	kJ/mol	Joback Method
hvap	63.59	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.658		Crippen Method
mcvol	194.630	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1739.00		NIST Webbook
tb	650.53	K	Joback Method
tc	836.12	K	Joback Method
tf	382.99	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.98	J/mol×K	650.53	Joback Method
cpg	536.26	J/mol×K	681.46	Joback Method
cpg	549.82	J/mol×K	712.39	Joback Method
cpg	562.66	J/mol×K	743.32	Joback Method
cpg	574.81	J/mol×K	774.25	Joback Method
cpg	586.28	J/mol×K	805.19	Joback Method
cpg	597.09	J/mol×K	836.12	Joback Method

Sources

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=U321678&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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