

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

Inchi: InChI=1S/C23H43NO3/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-27-23(26)19-20-2
InchiKey: IIEDWJAFEVXBQS-UHFFFAOYSA-N
Formula: C23H43NO3
SMILES: C=CC(=O)NCCC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 381.59

Physical Properties

Property code	Value	Unit	Source
gf	-42.83	kJ/mol	Joback Method
hf	-696.53	kJ/mol	Joback Method
hfus	63.53	kJ/mol	Joback Method
hvap	88.46	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	6.093		Crippen Method
mvol	349.620	ml/mol	McGowan Method
pc	939.79	kPa	Joback Method
rinpol	2937.00		NIST Webbook
rinpol	2937.00		NIST Webbook
tb	902.65	K	Joback Method
tc	1105.55	K	Joback Method
tf	521.96	K	Joback Method
vc	1.369	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1159.45	J/mol×K	902.65	Joback Method
cpg	1178.44	J/mol×K	936.47	Joback Method
cpg	1196.21	J/mol×K	970.28	Joback Method
cpg	1212.79	J/mol×K	1004.10	Joback Method
cpg	1228.23	J/mol×K	1037.92	Joback Method
cpg	1242.60	J/mol×K	1071.73	Joback Method
cpg	1255.93	J/mol×K	1105.55	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U321686&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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