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

Inchi: InChI=1S/C24H45NO3/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-28-24(27)20-2
InchiKey: OEKXWVFTOJXFIN-UHFFFAOYSA-N
Formula: C24H45NO3
SMILES: C=CC(=O)NCCC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 395.62

Physical Properties

Property code	Value	Unit	Source
gf	-34.41	kJ/mol	Joback Method
hf	-717.17	kJ/mol	Joback Method
hfus	66.12	kJ/mol	Joback Method
hvap	90.69	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	6.483		Crippen Method
mcvol	363.710	ml/mol	McGowan Method
pc	886.83	kPa	Joback Method
rinpol	3048.00		NIST Webbook
rinpol	3048.00		NIST Webbook
tb	925.53	K	Joback Method
tc	1135.03	K	Joback Method
tf	533.23	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1222.29	J/mol×K	925.53	Joback Method
cpg	1241.86	J/mol×K	960.45	Joback Method
cpg	1260.10	J/mol×K	995.36	Joback Method
cpg	1277.08	J/mol×K	1030.28	Joback Method
cpg	1292.85	J/mol×K	1065.20	Joback Method
cpg	1307.47	J/mol×K	1100.11	Joback Method
cpg	1320.99	J/mol×K	1135.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321687&Units=SI
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

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