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

Inchi: InChI=1S/C16H29NO3/c1-3-5-6-7-8-9-10-11-14-20-16(19)12-13-17-15(18)4-2/h4H,2-3,5-
InchiKey: ZUNFPBSVDQJZOJ-UHFFFAOYSA-N
Formula: C16H29NO3
SMILES: C=CC(=O)NCCC(=O)OCCCCCCCCCC
Mol. weight [g/mol]: 283.41

Physical Properties

Property code	Value	Unit	Source
gf	-101.77	kJ/mol	Joback Method
hf	-552.05	kJ/mol	Joback Method
hfus	45.40	kJ/mol	Joback Method
hvap	72.88	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.363		Crippen Method
mcvol	250.990	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
rinpol	2204.00		NIST Webbook
tb	742.49	K	Joback Method
tc	923.71	K	Joback Method
tf	443.07	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.62	J/mol×K	742.49	Joback Method
cpg	755.50	J/mol×K	772.69	Joback Method
cpg	770.54	J/mol×K	802.90	Joback Method
cpg	784.76	J/mol×K	833.10	Joback Method
cpg	798.20	J/mol×K	863.31	Joback Method
cpg	810.87	J/mol×K	893.51	Joback Method
cpg	822.78	J/mol×K	923.71	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=U321681&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