«beta»-Alanine, N-capryloyl-, heptyl ester

Inchi: InChI=1S/C18H35NO3/c1-3-5-7-9-11-13-17(20)19-15-14-18(21)22-16-12-10-8-6-4-2/h3-1
InchiKey: JVKNDDADIRYROV-UHFFFAOYSA-N
Formula: C18H35NO3
SMILES: CCCCCCCOC(=O)CCNC(=O)CCCCCCC
Mol. weight [g/mol]: 313.48

Physical Properties

Property code	Value	Unit	Source
gf	-172.77	kJ/mol	Joback Method
hf	-718.76	kJ/mol	Joback Method
hfus	51.86	kJ/mol	Joback Method
hvap	78.00	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.367		Crippen Method
mcvol	283.470	ml/mol	McGowan Method
pc	1253.92	kPa	Joback Method
rinpol	2375.00		NIST Webbook
tb	791.57	K	Joback Method
tc	974.52	K	Joback Method
tf	467.37	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.76	J/mol×K	791.57	Joback Method
cpg	898.99	J/mol×K	822.06	Joback Method
cpg	915.26	J/mol×K	852.55	Joback Method
cpg	930.62	J/mol×K	883.05	Joback Method
cpg	945.08	J/mol×K	913.54	Joback Method
cpg	958.66	J/mol×K	944.03	Joback Method
cpg	971.39	J/mol×K	974.52	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=U321813&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