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

Inchi: InChI=1S/C17H33NO3/c1-3-5-7-9-10-12-16(19)18-14-13-17(20)21-15-11-8-6-4-2/h3-15H
InchiKey: ZXXXYWWYQSXQLR-UHFFFAOYSA-N
Formula: C17H33NO3
SMILES: CCCCCCCC(=O)NCCC(=O)OCCCCCC
Mol. weight [g/mol]: 299.45

Physical Properties

Property code	Value	Unit	Source
gf	-181.19	kJ/mol	Joback Method
hf	-698.12	kJ/mol	Joback Method
hfus	49.27	kJ/mol	Joback Method
hvap	75.77	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.977		Crippen Method
mcvol	269.380	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
rinpol	2278.00		NIST Webbook
tb	768.69	K	Joback Method
tc	949.75	K	Joback Method
tf	456.10	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.82	J/mol×K	768.69	Joback Method
cpg	839.64	J/mol×K	798.87	Joback Method
cpg	855.55	J/mol×K	829.04	Joback Method
cpg	870.59	J/mol×K	859.22	Joback Method
cpg	884.78	J/mol×K	889.40	Joback Method
cpg	898.13	J/mol×K	919.58	Joback Method
cpg	910.67	J/mol×K	949.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321812&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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