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

Inchi: InChI=1S/C15H29NO3/c1-3-5-7-9-13-19-15(18)11-12-16-14(17)10-8-6-4-2/h3-13H2,1-2H
InchiKey: FOTFIIGLERIXMU-UHFFFAOYSA-N
Formula: C15H29NO3
SMILES: CCCCCCOC(=O)CCNC(=O)CCCCC
Mol. weight [g/mol]: 271.40

Physical Properties

Property code	Value	Unit	Source
gf	-198.03	kJ/mol	Joback Method
hf	-656.84	kJ/mol	Joback Method
hfus	44.09	kJ/mol	Joback Method
hvap	71.32	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.196		Crippen Method
mcvol	241.200	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	2071.00		NIST Webbook
rinpol	2071.00		NIST Webbook
tb	722.93	K	Joback Method
tc	902.08	K	Joback Method
tf	433.56	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.90	J/mol×K	722.93	Joback Method
cpg	723.89	J/mol×K	752.79	Joback Method
cpg	739.06	J/mol×K	782.65	Joback Method
cpg	753.44	J/mol×K	812.50	Joback Method
cpg	767.04	J/mol×K	842.36	Joback Method
cpg	779.88	J/mol×K	872.22	Joback Method
cpg	791.98	J/mol×K	902.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321783&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