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

Inchi: InChI=1S/C14H27NO3/c1-3-5-7-9-13(16)15-11-10-14(17)18-12-8-6-4-2/h3-12H2,1-2H3,(
InchiKey: ZJHMBJNSDPHOEA-UHFFFAOYSA-N
Formula: C14H27NO3
SMILES: CCCCCOC(=O)CCNC(=O)CCCCC
Mol. weight [g/mol]: 257.37

Physical Properties

Property code	Value	Unit	Source
gf	-206.45	kJ/mol	Joback Method
hf	-636.20	kJ/mol	Joback Method
hfus	41.50	kJ/mol	Joback Method
hvap	69.10	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	2.806		Crippen Method
mcvol	227.110	ml/mol	McGowan Method
pc	1679.66	kPa	Joback Method
rinpol	1972.00		NIST Webbook
tb	700.05	K	Joback Method
tc	879.07	K	Joback Method
tf	422.29	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.07	J/mol×K	700.05	Joback Method
cpg	667.62	J/mol×K	729.89	Joback Method
cpg	682.40	J/mol×K	759.72	Joback Method
cpg	696.42	J/mol×K	789.56	Joback Method
cpg	709.69	J/mol×K	819.39	Joback Method
cpg	722.24	J/mol×K	849.23	Joback Method
cpg	734.07	J/mol×K	879.07	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=U321782&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

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