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

Inchi: InChI=1S/C13H25NO3/c1-3-5-6-7-8-9-12(15)14-11-10-13(16)17-4-2/h3-11H2,1-2H3,(H,1
InchiKey: RVFHTSWLFYIGIP-UHFFFAOYSA-N
Formula: C13H25NO3
SMILES: CCCCCCCC(=O)NCCC(=O)OCC
Mol. weight [g/mol]: 243.34

Physical Properties

Property code	Value	Unit	Source
gf	-214.87	kJ/mol	Joback Method
hf	-615.56	kJ/mol	Joback Method
hfus	38.91	kJ/mol	Joback Method
hvap	66.87	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.416		Crippen Method
mcvol	213.020	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	1883.00		NIST Webbook
rinpol	1883.00		NIST Webbook
tb	677.17	K	Joback Method
tc	856.53	K	Joback Method
tf	411.02	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.44	J/mol×K	677.17	Joback Method
cpg	612.52	J/mol×K	707.06	Joback Method
cpg	626.87	J/mol×K	736.96	Joback Method
cpg	640.50	J/mol×K	766.85	Joback Method
cpg	653.42	J/mol×K	796.74	Joback Method
cpg	665.64	J/mol×K	826.64	Joback Method
cpg	677.17	J/mol×K	856.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321806&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