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

Inchi: InChI=1S/C11H21NO3/c1-3-5-6-7-10(13)12-9-8-11(14)15-4-2/h3-9H2,1-2H3,(H,12,13)
InchiKey: CIQIHYXHUNFHDW-UHFFFAOYSA-N
Formula: C11H21NO3
SMILES: CCCCCC(=O)NCCC(=O)OCC
Mol. weight [g/mol]: 215.29

Physical Properties

Property code	Value	Unit	Source
gf	-231.71	kJ/mol	Joback Method
hf	-574.28	kJ/mol	Joback Method
hfus	33.73	kJ/mol	Joback Method
hvap	62.42	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.636		Crippen Method
mcvol	184.840	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinpol	1673.00		NIST Webbook
rinpol	1673.00		NIST Webbook
tb	631.41	K	Joback Method
tc	812.70	K	Joback Method
tf	388.48	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.13	J/mol×K	631.41	Joback Method
cpg	506.14	J/mol×K	661.63	Joback Method
cpg	519.50	J/mol×K	691.84	Joback Method
cpg	532.20	J/mol×K	722.06	Joback Method
cpg	544.27	J/mol×K	752.27	Joback Method
cpg	555.70	J/mol×K	782.49	Joback Method
cpg	566.52	J/mol×K	812.70	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=U321779&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