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

Inchi: InChI=1S/C12H23NO3/c1-3-5-6-7-11(14)13-9-8-12(15)16-10-4-2/h3-10H2,1-2H3,(H,13,1
InchiKey: OGPRBKDKHWXZFR-UHFFFAOYSA-N
Formula: C12H23NO3
SMILES: CCCCCC(=O)NCCC(=O)OCCC
Mol. weight [g/mol]: 229.32

Physical Properties

Property code	Value	Unit	Source
gf	-223.29	kJ/mol	Joback Method
hf	-594.92	kJ/mol	Joback Method
hfus	36.32	kJ/mol	Joback Method
hvap	64.64	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.026		Crippen Method
mcvol	198.930	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1768.00		NIST Webbook
tb	654.29	K	Joback Method
tc	834.43	K	Joback Method
tf	399.75	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.10	J/mol×K	654.29	Joback Method
cpg	558.67	J/mol×K	684.31	Joback Method
cpg	572.55	J/mol×K	714.34	Joback Method
cpg	585.74	J/mol×K	744.36	Joback Method
cpg	598.26	J/mol×K	774.38	Joback Method
cpg	610.11	J/mol×K	804.41	Joback Method
cpg	621.31	J/mol×K	834.43	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=U321780&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