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

Inchi: InChI=1S/C21H41NO3/c1-3-5-7-8-9-10-11-12-13-15-19-25-21(24)17-18-22-20(23)16-14-
InchiKey: IMSGXGLJUNOYDQ-UHFFFAOYSA-N
Formula: C21H41NO3
SMILES: CCCCCCCCCCCCOC(=O)CCNC(=O)CCCCC
Mol. weight [g/mol]: 355.56

Physical Properties

Property code	Value	Unit	Source
gf	-147.51	kJ/mol	Joback Method
hf	-780.68	kJ/mol	Joback Method
hfus	59.63	kJ/mol	Joback Method
hvap	84.68	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.537		Crippen Method
mcvol	325.740	ml/mol	McGowan Method
pc	1032.57	kPa	Joback Method
rinpol	2682.00		NIST Webbook
tb	860.21	K	Joback Method
tc	1053.29	K	Joback Method
tf	501.18	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.60	J/mol×K	860.21	Joback Method
cpg	1082.15	J/mol×K	892.39	Joback Method
cpg	1099.57	J/mol×K	924.57	Joback Method
cpg	1115.89	J/mol×K	956.75	Joback Method
cpg	1131.16	J/mol×K	988.93	Joback Method
cpg	1145.39	J/mol×K	1021.11	Joback Method
cpg	1158.63	J/mol×K	1053.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321788&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