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

Inchi: InChI=1S/C25H49NO3/c1-3-5-7-9-10-11-12-13-14-15-17-19-23-29-25(28)21-22-26-24(27
InchiKey: MIOJYJLNVXRQAJ-UHFFFAOYSA-N
Formula: C25H49NO3
SMILES: CCCCCCCCCCCCCCOC(=O)CCNC(=O)CCCCCCC
Mol. weight [g/mol]: 411.66

Physical Properties

Property code	Value	Unit	Source
gf	-113.83	kJ/mol	Joback Method
hf	-863.24	kJ/mol	Joback Method
hfus	69.99	kJ/mol	Joback Method
hvap	93.58	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.097		Crippen Method
mcvol	382.100	ml/mol	McGowan Method
pc	818.20	kPa	Joback Method
rinpol	3280.00		NIST Webbook
tb	951.73	K	Joback Method
tc	1171.22	K	Joback Method
tf	546.26	K	Joback Method
vc	1.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.38	J/mol×K	951.73	Joback Method
cpg	1336.20	J/mol×K	988.31	Joback Method
cpg	1355.50	J/mol×K	1024.89	Joback Method
cpg	1373.33	J/mol×K	1061.48	Joback Method
cpg	1389.75	J/mol×K	1098.06	Joback Method
cpg	1404.85	J/mol×K	1134.64	Joback Method
cpg	1418.67	J/mol×K	1171.22	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=U321818&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