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

Inchi: InChI=1S/C24H47NO3/c1-3-5-7-8-9-10-11-12-13-14-15-16-18-22-28-24(27)20-21-25-23(
InchiKey: SKUCVAYUGSXBBO-UHFFFAOYSA-N
Formula: C24H47NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCNC(=O)CCCCC
Mol. weight [g/mol]: 397.63

Physical Properties

Property code	Value	Unit	Source
gf	-122.25	kJ/mol	Joback Method
hf	-842.60	kJ/mol	Joback Method
hfus	67.40	kJ/mol	Joback Method
hvap	91.36	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	6.707		Crippen Method
mcvol	368.010	ml/mol	McGowan Method
pc	865.05	kPa	Joback Method
rinpol	3095.00		NIST Webbook
rinpol	3095.00		NIST Webbook
tb	928.85	K	Joback Method
tc	1140.13	K	Joback Method
tf	534.99	K	Joback Method
vc	1.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1251.61	J/mol×K	928.85	Joback Method
cpg	1271.79	J/mol×K	964.06	Joback Method
cpg	1290.57	J/mol×K	999.28	Joback Method
cpg	1307.99	J/mol×K	1034.49	Joback Method
cpg	1324.11	J/mol×K	1069.70	Joback Method
cpg	1338.99	J/mol×K	1104.91	Joback Method
cpg	1352.67	J/mol×K	1140.13	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321790&Units=SI

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