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

Inchi: InChI=1S/C24H45NO3/c1-2-3-4-5-6-7-8-9-10-11-12-16-21-28-23(26)19-20-25-24(27)22-
InchiKey: BGFKYKHYNJJJNI-UHFFFAOYSA-N
Formula: C24H45NO3
SMILES: CCCCCCCCCCCCCCOC(=O)CCNC(=O)C1CCCCC1
Mol. weight [g/mol]: 395.62

Physical Properties

Property code	Value	Unit	Source
gf	-97.80	kJ/mol	Joback Method
hf	-788.28	kJ/mol	Joback Method
hfus	59.24	kJ/mol	Joback Method
hvap	91.78	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.317		Crippen Method
mcvol	357.150	ml/mol	McGowan Method
pc	979.62	kPa	Joback Method
rinpol	3250.00		NIST Webbook
rinpol	3250.00		NIST Webbook
tb	948.40	K	Joback Method
tc	1161.11	K	Joback Method
tf	542.37	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1248.50	J/mol×K	948.40	Joback Method
cpg	1267.75	J/mol×K	983.85	Joback Method
cpg	1285.48	J/mol×K	1019.30	Joback Method
cpg	1301.73	J/mol×K	1054.75	Joback Method
cpg	1316.57	J/mol×K	1090.21	Joback Method
cpg	1330.06	J/mol×K	1125.66	Joback Method
cpg	1342.26	J/mol×K	1161.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321969&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