

DL-Alanine, N-methyl-N-(2-ethylhexyloxycarbonyl)-, heptadecyl ester

InChI: InChI=1S/C30H59NO4/c1-6-9-11-12-13-14-15-16-17-18-19-20-21-22-23-25-34-29(32)27
InChIKey: UFZSAZSEOIWYRI-UHFFFAOYSA-N

Formula: C30H59NO4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 497.79

Physical Properties

Property code	Value	Unit	Source
gf	-160.22	kJ/mol	Joback Method
hf	-1095.16	kJ/mol	Joback Method
hfus	75.00	kJ/mol	Joback Method
hvap	101.95	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	9.074		Crippen Method
mvol	458.420	ml/mol	McGowan Method
pc	627.51	kPa	Joback Method
rinpol	3178.00		NIST Webbook
rinpol	3178.00		NIST Webbook
tb	1049.94	K	Joback Method
tc	1319.00	K	Joback Method
tf	574.65	K	Joback Method
vc	1.770	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1651.20	J/molxK	1049.94	Joback Method
cpg	1675.29	J/molxK	1094.78	Joback Method
cpg	1696.85	J/molxK	1139.63	Joback Method
cpg	1716.00	J/molxK	1184.47	Joback Method
cpg	1732.89	J/molxK	1229.31	Joback Method
cpg	1747.65	J/molxK	1274.16	Joback Method
cpg	1760.41	J/molxK	1319.00	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U392668&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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