DL-Alanine, N-methyl-N-decyloxycarbonyl-, hexadecyl ester

Inchi: InChI=1S/C31H61NO4/c1-5-7-9-11-13-15-16-17-18-19-20-22-23-25-27-35-30(33)29(3)32
InchiKey: XZOHMLYDERJNAH-UHFFFAOYSA-N
Formula: C31H61NO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCCCCCCC
Mol. weight [g/mol]: 511.82

Physical Properties

Property code	Value	Unit	Source
gf	-149.36	kJ/mol	Joback Method
hf	-1110.52	kJ/mol	Joback Method
hfus	81.12	kJ/mol	Joback Method
hvap	104.57	kJ/mol	Joback Method
log10ws	-10.18		Crippen Method
logp	9.608		Crippen Method
mcvol	472.510	ml/mol	McGowan Method
pc	596.05	kPa	Joback Method
rinpol	3357.00		NIST Webbook
rinpol	3357.00		NIST Webbook
tb	1073.26	K	Joback Method
tc	1362.40	K	Joback Method
tf	600.92	K	Joback Method
vc	1.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1716.79	J/mol×K	1073.26	Joback Method
cpg	1742.18	J/mol×K	1121.45	Joback Method
cpg	1764.69	J/mol×K	1169.64	Joback Method
cpg	1784.49	J/mol×K	1217.83	Joback Method
cpg	1801.77	J/mol×K	1266.02	Joback Method
cpg	1816.70	J/mol×K	1314.21	Joback Method
cpg	1829.47	J/mol×K	1362.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392686&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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