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

Inchi: InChI=1S/C30H59NO4/c1-5-7-9-11-13-15-16-17-18-19-21-22-24-26-34-29(32)28(3)31(4)

InchiKey: CHHZCWVJTSURLT-UHFFFAOYSA-N

Formula: C30H59NO4

SMILES: CCCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCCCCCCC

Mol. weight [g/mol]: 497.79

Physical Properties

Property code	Value	Unit	Source
gf	-157.78	kJ/mol	Joback Method
hf	-1089.88	kJ/mol	Joback Method
hfus	78.53	kJ/mol	Joback Method
hvap	102.34	kJ/mol	Joback Method
log10ws	-9.77		Crippen Method
logp	9.218		Crippen Method
mcvol	458.420	ml/mol	McGowan Method
pc	625.00	kPa	Joback Method
rinpol	3254.00		NIST Webbook
rinpol	3254.00		NIST Webbook
tb	1050.38	K	Joback Method
tc	1323.14	K	Joback Method
tf	589.65	K	Joback Method
vc	1.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1651.02	J/mol×K	1050.38	Joback Method
cpg	1675.53	J/mol×K	1095.84	Joback Method
cpg	1697.44	J/mol×K	1141.30	Joback Method
cpg	1716.92	J/mol×K	1186.76	Joback Method
cpg	1734.09	J/mol×K	1232.22	Joback Method
cpg	1749.11	J/mol×K	1277.68	Joback Method
cpg	1762.11	J/mol×K	1323.14	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=U392685&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