

DL-Alanine, N-methyl-N-octyloxycarbonyl-, dodecyl ester

Inchi:	InChI=1S/C25H49NO4/c1-5-7-9-11-13-14-15-16-18-19-21-29-24(27)23(3)26(4)25(28)30-
InchiKey:	FBYWCEQVDODKSV-UHFFFAOYSA-N
Formula:	C25H49NO4
SMILES:	CCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCCCCC
Mol. weight [g/mol]:	427.66

Physical Properties

Property code	Value	Unit	Source
gf	-199.88	kJ/mol	Joback Method
hf	-986.68	kJ/mol	Joback Method
hfus	65.58	kJ/mol	Joback Method
hvap	91.21	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	7.268		Crippen Method
mcvol	387.970	ml/mol	McGowan Method
pc	807.08	kPa	Joback Method
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook
tb	935.98	K	Joback Method
tc	1150.48	K	Joback Method
tf	533.30	K	Joback Method
vc	1.496	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1326.39	J/molxK	935.98	Joback Method
cpg	1347.30	J/molxK	971.73	Joback Method
cpg	1366.62	J/molxK	1007.48	Joback Method
cpg	1384.40	J/molxK	1043.23	Joback Method
cpg	1400.70	J/molxK	1078.98	Joback Method
cpg	1415.56	J/molxK	1114.73	Joback Method
cpg	1429.05	J/molxK	1150.48	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=U392654&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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