

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

Inchi:	InChI=1S/C27H53NO4/c1-5-7-9-11-13-15-16-18-19-21-23-31-26(29)25(3)28(4)27(30)32
InchiKey:	DEWOYAXWLZQSFC-UHFFFAOYSA-N
Formula:	C27H53NO4
SMILES:	CCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCCCCCC
Mol. weight [g/mol]:	455.71

Physical Properties

Property code	Value	Unit	Source
gf	-183.04	kJ/mol	Joback Method
hf	-1027.96	kJ/mol	Joback Method
hfus	70.76	kJ/mol	Joback Method
hvap	95.66	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	8.048		Crippen Method
mvol	416.150	ml/mol	McGowan Method
pc	725.75	kPa	Joback Method
rinpol	2940.00		NIST Webbook
rinpol	2940.00		NIST Webbook
tb	981.74	K	Joback Method
tc	1215.30	K	Joback Method
tf	555.84	K	Joback Method
vc	1.607	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1455.24	J/molxK	981.74	Joback Method
cpg	1477.43	J/molxK	1020.67	Joback Method
cpg	1497.70	J/molxK	1059.59	Joback Method
cpg	1516.15	J/molxK	1098.52	Joback Method
cpg	1532.85	J/molxK	1137.44	Joback Method
cpg	1547.86	J/molxK	1176.37	Joback Method
cpg	1561.28	J/molxK	1215.30	Joback Method

Sources

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=U392682&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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