

DL-Alanine, N-methyl-N-(3-chloro-2-methylpropoxycarbonyl)-, nonyl ester

InChI: InChI=1S/C18H34ClNO4/c1-5-6-7-8-9-10-11-12-23-17(21)16(3)20(4)18(22)24-14-15(2)1
InChIKey: ZBJLSHKQGQNBMB-UHFFFAOYSA-N

Formula: C18H34ClNO4

SMILES: CCCCCCCCOC(=O)C(C)N(C)C(=O)OCC(C)CCI

Mol. weight [g/mol]: 363.92

Physical Properties

Property code	Value	Unit	Source
gf	-273.19	kJ/mol	Joback Method
hf	-863.22	kJ/mol	Joback Method
hfus	48.12	kJ/mol	Joback Method
hvap	79.63	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.612		Crippen Method
mcvol	301.580	ml/mol	McGowan Method
pc	1208.15	kPa	Joback Method
rinpol	2208.00		NIST Webbook
rinpol	2208.00		NIST Webbook
tb	812.81	K	Joback Method
tc	1000.66	K	Joback Method
tf	469.33	K	Joback Method
vc	1.147	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.62	J/molxK	812.81	Joback Method
cpg	941.47	J/molxK	844.12	Joback Method
cpg	957.29	J/molxK	875.43	Joback Method
cpg	972.09	J/molxK	906.73	Joback Method
cpg	985.90	J/molxK	938.04	Joback Method
cpg	998.73	J/molxK	969.35	Joback Method
cpg	1010.62	J/molxK	1000.66	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U392771&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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