

D-Alanine, N-ethoxycarbonyl-, tridecyl ester

Inchi:	InChI=1S/C19H37NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-24-18(21)17(3)20-19(22)23-5
InchiKey:	WMDYZDVTHXVWPA-UHFFFAOYSA-N
Formula:	C19H37NO4
SMILES:	CCCCCCCCCCCCCOC(=O)C(C)N=C(O)OCC
Mol. weight [g/mol]:	343.50

Physical Properties

Property code	Value	Unit	Source
hf	-897.59	kJ/mol	Joback Method
hvap	89.14	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.180		Crippen Method
mcvol	303.430	ml/mol	McGowan Method
pc	1101.54	kPa	Joback Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	901.13	K	Joback Method
tc	1103.27	K	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=U347756&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation 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

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