

D-Alanine, N-ethoxycarbonyl-, isohexyl ester

Inchi:	InChI=1S/C12H23NO4/c1-5-16-12(15)13-10(4)11(14)17-8-6-7-9(2)3/h9-10H,5-8H2,1-4H1
InchiKey:	QVNNZMLPTQZXQR-UHFFFAOYSA-N
Formula:	C12H23NO4
SMILES:	CCOC(O)=NC(C)C(=O)OCCCC(C)C
Mol. weight [g/mol]:	245.32

Physical Properties

Property code	Value	Unit	Source
hf	-758.39	kJ/mol	Joback Method
hvap	73.17	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.305		Crippen Method
mcvol	204.800	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
rinpol	1603.00		NIST Webbook
rinpol	1603.00		NIST Webbook
tb	740.53	K	Joback Method
tc	927.24	K	Joback Method

Sources

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=U347748&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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