

D-Alanine, N-butoxycarbonyl-, butyl ester

Inchi: InChI=1S/C12H23NO4/c1-4-6-8-16-11(14)10(3)13-12(15)17-9-7-5-2/h10H,4-9H2,1-3H3,
InchiKey: OZMOOZXSSWWOTM-UHFFFAOYSA-N
Formula: C12H23NO4
SMILES: CCCCOC(=O)C(C)N=C(O)OCCCC
Mol. weight [g/mol]: 245.32

Physical Properties

Property code	Value	Unit	Source
hf	-753.11	kJ/mol	Joback Method
hvap	73.56	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.449		Crippen Method
mcvol	204.800	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
rinpol	1667.00		NIST Webbook
rinpol	1667.00		NIST Webbook
tb	740.97	K	Joback Method
tc	925.58	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=U347718&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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