

D-Alanine, N-butoxycarbonyl-, tridecyl ester

Inchi: InChI=1S/C21H41NO4/c1-4-6-8-9-10-11-12-13-14-15-16-18-25-20(23)19(3)22-21(24)26
InchiKey: WTNHRUBZHLSY-UHFFFAOYSA-N
Formula: C21H41NO4
SMILES: CCCCCCCCCCCCCOC(=O)C(C)N=C(O)OCCCC
Mol. weight [g/mol]: 371.55

Physical Properties

Property code	Value	Unit	Source
hf	-938.87	kJ/mol	Joback Method
hvap	93.59	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	5.960		Crippen Method
mcvol	331.610	ml/mol	McGowan Method
pc	973.52	kPa	Joback Method
rinpol	2515.00		NIST Webbook
rinpol	2515.00		NIST Webbook
tb	946.89	K	Joback Method
tc	1161.84	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U347727&Units=SI>

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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