

D-Alanine, N-allyloxycarbonyl-, pentadecyl ester

Inchi: InChI=1S/C22H41NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-19-26-21(24)20(3)23-22(2)
InchiKey: IJVRWUDUIAVXSM-UHFFFAOYSA-N
Formula: C22H41NO4
SMILES: C=CCOC(O)=NC(C)C(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 383.57

Physical Properties

Property code	Value	Unit	Source
hf	-834.08	kJ/mol	Joback Method
hvap	95.15	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	6.126		Crippen Method
mcvol	341.400	ml/mol	McGowan Method
pc	941.52	kPa	Joback Method
rinpol	2614.00		NIST Webbook
rinpol	2614.00		NIST Webbook
tb	966.45	K	Joback Method
tc	1187.24	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=U347738&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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