

1-Aminocyclopentanecarboxylic acid, N-(but-2-yn-1-yloxycarbonyl)-, dodecyl ester

Inchi: InChI=1S/C23H39NO4/c1-3-5-7-8-9-10-11-12-13-16-20-27-21(25)23(17-14-15-18-23)24
InchiKey: IDXDSJVAUUOBPJ-UHFFFAOYSA-N
Formula: C23H39NO4
SMILES: CC#CCOC(O)=NC1(C(=O)OCCCCCCCCCCCC)CCCC1
Mol. weight [g/mol]: 393.56

Physical Properties

Property code	Value	Unit	Source
hf	-626.85	kJ/mol	Joback Method
hvap	99.69	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	5.717		Crippen Method
mcvol	340.330	ml/mol	McGowan Method
pc	1096.44	kPa	Joback Method
rinpol	2770.00		NIST Webbook
tb	1017.61	K	Joback Method
tc	1245.86	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=U392586&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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