

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

Inchi: InChI=1S/C24H41NO4/c1-3-5-7-8-9-10-11-12-13-14-17-21-28-22(26)24(18-15-16-19-24)
InchiKey: RJWDCVKPIQILII-UHFFFAOYSA-N
Formula: C24H41NO4
SMILES: CC#CCOC(O)=NC1(C(=O)OCCCCCCCCCCCCC)CCCC1
Mol. weight [g/mol]: 407.59

Physical Properties

Property code	Value	Unit	Source
hf	-647.49	kJ/mol	Joback Method
hvap	101.91	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	6.107		Crippen Method
mcvol	354.420	ml/mol	McGowan Method
pc	1029.92	kPa	Joback Method
rinpol	2866.00		NIST Webbook
rinpol	2866.00		NIST Webbook
tb	1040.49	K	Joback Method
tc	1274.64	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=U392587&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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