

1-Aminocyclopentanecarboxylic acid, N-(but-3-yn-1-yloxycarbonyl)-, nonyl ester

Inchi: InChI=1S/C20H33NO4/c1-3-5-7-8-9-10-13-17-24-18(22)20(14-11-12-15-20)21-19(23)25-
InchiKey: JKZHWGYDAGEBRR-UHFFFAOYSA-N
Formula: C20H33NO4
SMILES: C#CCCOC(O)=NC1(C(=O)OCCCCCCCCC)CCCC1
Mol. weight [g/mol]: 351.48

Physical Properties

Property code	Value	Unit	Source
hf	-545.33	kJ/mol	Joback Method
hvap	90.72	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.547		Crippen Method
mcvol	298.060	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
rinsol	2391.00		NIST Webbook
rinsol	2391.00		NIST Webbook
tb	930.09	K	Joback Method
tc	1141.86	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=U392572&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

Latest version available from:

<https://www.cheméo.com/cid/96-521-7/1-Aminocyclopentanecarboxylic-acid-N-but-3-yn-1-yloxycarbonyl-nonyl-ester.>

Generated by Cheméo on 2024-04-26 06:40:15.352323688 +0000 UTC m=+16402864.272900999.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.