

2-Aminopent-4-enoic acid, N-octyloxycarbonyl-, butyl ester

Inchi: InChI=1S/C18H33NO4/c1-4-7-9-10-11-12-15-23-18(21)19-16(13-6-3)17(20)22-14-8-5-2/
InchiKey: MCWZHAIQNSKPHW-UHFFFAOYSA-N
Formula: C18H33NO4
SMILES: C=CCC(N=C(O)OCCCCCCCC)C(=O)OCCCC
Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
hf	-751.52	kJ/mol	Joback Method
hvap	86.24	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.566		Crippen Method
mcvol	285.040	ml/mol	McGowan Method
pc	1209.83	kPa	Joback Method
rinpol	2147.00		NIST Webbook
rinpol	2147.00		NIST Webbook
tb	874.93	K	Joback Method
tc	1071.85	K	Joback Method

Sources

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=U393151&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/99-357-7/2-Aminopent-4-enoic-acid-N-octyloxycarbonyl-butyl-ester.pdf>

Generated by Cheméo on 2024-05-03 11:14:24.625033467 +0000 UTC m=+17024113.545610782.

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