

2-Aminopent-4-enoic acid, N-(2-benzyloxyetoxycarbonyl)-, octyl ester

Inchi: InChI=1S/C23H35NO5/c1-3-5-6-7-8-12-16-28-22(25)21(13-4-2)24-23(26)29-18-17-27-19
InchiKey: RXPYMLXHWMWTMI-UHFFFAOYSA-N
Formula: C23H35NO5
SMILES: C=CCC(N=C(O)OCCOCc1ccccc1)C(=O)OCCCCCCCC
Mol. weight [g/mol]: 405.53

Physical Properties

Property code	Value	Unit	Source
hf	-750.41	kJ/mol	Joback Method
hvap	102.06	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.982		Crippen Method
mcvol	337.600	ml/mol	McGowan Method
pc	1081.35	kPa	Joback Method
rinpol	2896.00		NIST Webbook
rinpol	2896.00		NIST Webbook
tb	1038.43	K	Joback Method
tc	1273.25	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=U393185&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/81-686-1/2-Aminopent-4-enoic-acid-N-2-benzyloxyetoxycarbonyl-octyl-ester.pdf>

Generated by Cheméo on 2024-05-06 02:42:16.168279905 +0000 UTC m=+17252585.088857217.

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