

2-Aminopent-4-enoic acid, N-vinyloxycarbonyl-, heptyl ester

Inchi: InChI=1S/C15H25NO4/c1-4-7-8-9-10-12-20-14(17)13(11-5-2)16-15(18)19-6-3/h5-6,13H,
InchiKey: UBDUKVGLDHQTAQ-UHFFFAOYSA-N
Formula: C15H25NO4
SMILES: C=CCC(N=C(O)OC=C)C(=O)OCCCCCCC
Mol. weight [g/mol]: 283.36

Physical Properties

Property code	Value	Unit	Source
hf	-564.17	kJ/mol	Joback Method
hvap	78.89	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.519		Crippen Method
mcvol	238.470	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpole	1883.00		NIST Webbook
rinpole	1883.00		NIST Webbook
tb	802.97	K	Joback Method
tc	992.56	K	Joback Method

Sources

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=U393211&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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