

«beta»-Alanine, N-allyloxycarbonyl-, octyl ester

Inchi:	InChI=1S/C15H27NO4/c1-3-5-6-7-8-9-13-19-14(17)10-11-16-15(18)20-12-4-2/h4H,2-3,5
InchiKey:	HCHFINCKDLABDU-UHFFFAOYSA-N
Formula:	C15H27NO4
SMILES:	C=CCOC(O)=NCCC(=O)OCCCCCCCC
Mol. weight [g/mol]:	285.38

Physical Properties

Property code	Value	Unit	Source
hf	-684.32	kJ/mol	Joback Method
hvap	79.95	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.397		Crippen Method
mcvol	242.770	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinpol	2055.00		NIST Webbook
rinpol	2055.00		NIST Webbook
tb	806.73	K	Joback Method
tc	994.03	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321036&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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