

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

Inchi: InChI=1S/C25H47NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-29-24(27)20-2
InchiKey: PXHVZZMAGXGDJ-UHFFFAOYSA-N
Formula: C25H47NO4
SMILES: C=CCOC(O)=NCCC(=O)OCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 425.64

Physical Properties

Property code	Value	Unit	Source
hf	-890.72	kJ/mol	Joback Method
hvap	102.21	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	7.298		Crippen Method
mcvol	383.670	ml/mol	McGowan Method
pc	791.26	kPa	Joback Method
rinpol	3242.00		NIST Webbook
rinpol	3242.00		NIST Webbook
tb	1035.53	K	Joback Method
tc	1289.28	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321045&Units=SI>
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>

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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