

«beta»-Alanine, N-caproyl-, hexadecyl ester

Inchi:	InChI=1S/C25H49NO3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-19-23-29-25(28)21-22-26
InchiKey:	AOPBQAXHUBWSPK-UHFFFAOYSA-N
Formula:	C25H49NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCN=C(O)CCCCC
Mol. weight [g/mol]:	411.66

Physical Properties

Property code	Value	Unit	Source
hf	-883.93	kJ/mol	Joback Method
hvap	100.47	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	7.938		Crippen Method
mcvol	382.100	ml/mol	McGowan Method
pc	780.25	kPa	Joback Method
rinpol	3286.00		NIST Webbook
rinpol	3286.00		NIST Webbook
tb	1016.43	K	Joback Method
tc	1262.66	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=U321791&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

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