

«beta»-Alanine, N-(3-methylbenzoyl)-, tetradecyl ester

Inchi:	InChI=1S/C25H41NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-20-29-24(27)18-19-26-25(28)23
InchiKey:	SSYWIVACJVMATO-UHFFFAOYSA-N
Formula:	C25H41NO3
SMILES:	CCCCCCCCCCCCCOC(=O)CCN=C(O)c1cccc(C)c1
Mol. weight [g/mol]:	403.60

Physical Properties

Property code	Value	Unit	Source
hf	-658.87	kJ/mol	Joback Method
hvap	103.41	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	6.934		Crippen Method
mcvol	358.340	ml/mol	McGowan Method
pc	938.64	kPa	Joback Method
tb	1048.09	K	Joback Method
tc	1288.23	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=U321636&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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