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

Inchi: InChI=1S/C23H37NO3/c1-3-4-5-6-7-8-9-10-11-12-18-27-22(25)16-17-24-23(26)21-15-13

InchiKey: MTPYCUFRBIWRFP-UHFFFAOYSA-N

Formula: C23H37NO3

SMILES: CCCCCCCCCCCCOC(=O)CCN=C(O)c1cccc(C)c1

Mol. weight [g/mol]: 375.54

Physical Properties

Property code	Value	Unit	Source
hf	-617.59	kJ/mol	Joback Method
hvap	98.96	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	6.154		Crippen Method
mcvol	330.160	ml/mol	McGowan Method
pc	1059.64	kPa	Joback Method
rinpol	3159.00		NIST Webbook
rinpol	3159.00		NIST Webbook
tb	1002.33	K	Joback Method
tc	1227.67	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=U321635&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature