«beta»-Alanine, N-(3-methoxybenzoyl)-, heptyl ester

Inchi: InChI=1S/C18H27NO4/c1-3-4-5-6-7-13-23-17(20)11-12-19-18(21)15-9-8-10-16(14-15)22

InchiKey: JQACRQIWEWZDOZ-UHFFFAOYSA-N

Formula: C18H27NO4

SMILES: CCCCCCCOC(=O)CCN=C(O)c1cccc(OC)c1

Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
hf	-646.61	kJ/mol	Joback Method
hvap	90.24	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.904		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
pc	1469.10	kPa	Joback Method
rinpol	2645.00		NIST Webbook
rinpol	2645.00		NIST Webbook
tb	910.35	K	Joback Method
tc	1119.26	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U321710&Units=SI

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