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

Inchi: InChI=1S/C20H31NO3/c1-3-4-5-6-7-8-9-15-24-19(22)13-14-21-20(23)18-12-10-11-17(2)

InchiKey: MWNDNIZWWQPUSM-UHFFFAOYSA-N

Formula: C20H31NO3

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

Mol. weight [g/mol]: 333.46

Physical Properties

Property code	Value	Unit	Source
hf	-555.67	kJ/mol	Joback Method
hvap	92.28	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.984		Crippen Method
mcvol	287.890	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	2722.00		NIST Webbook
rinpol	2722.00		NIST Webbook
tb	933.69	K	Joback Method
tc	1145.10	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321632&Units=SI

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

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