«beta»-Alanine, N-(1-naphthoyl)-, octyl ester

Inchi: InChI=1S/C22H29NO3/c1-2-3-4-5-6-9-17-26-21(24)15-16-23-22(25)20-14-10-12-18-11-7
InchiKey: YMABQZKZJPTCBJ-UHFFFAOYSA-N
Formula: C22H29NO3
SMILES: CCCCCCCCOC(=O)CCN=C(O)c1cccc2ccccc12
Mol. weight [g/mol]: 355.47

Physical Properties

Property code	Value	Unit	Source
hf	-405.88	kJ/mol	Joback Method
hvap	98.37	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.438		Crippen Method
mcvol	296.610	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	3213.00		NIST Webbook
rinpol	3213.00		NIST Webbook
tb	998.43	K	Joback Method
tc	1223.88	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321950&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