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

Inchi: InChI=1S/C24H33NO3/c1-2-3-4-5-6-7-8-11-19-28-23(26)17-18-25-24(27)22-16-12-14-20
InchiKey: JIEWLVMASXISDZ-UHFFFAOYSA-N
Formula: C24H33NO3
SMILES: CCCCCCCCCCOC(=O)CCN=C(O)c1cccc2ccccc12
Mol. weight [g/mol]: 383.52

Physical Properties

Property code	Value	Unit	Source
hf	-447.16	kJ/mol	Joback Method
hvap	102.82	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	6.218		Crippen Method
mcvol	324.790	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
tb	1044.19	K	Joback Method
tc	1278.44	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321952&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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