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

Inchi: InChI=1S/C19H23NO3/c1-2-3-6-14-23-18(21)12-13-20-19(22)17-11-7-9-15-8-4-5-10-16(
InchiKey: RULLWQMUNZCPFX-UHFFFAOYSA-N
Formula: C19H23NO3
SMILES: CCCCCOC(=O)CCN=C(O)c1cccc2ccccc12
Mol. weight [g/mol]: 313.39

Physical Properties

Property code	Value	Unit	Source
hf	-343.96	kJ/mol	Joback Method
hvap	91.69	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.268		Crippen Method
mcvol	254.340	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	2756.00		NIST Webbook
rinpol	2756.00		NIST Webbook
tb	929.79	K	Joback Method
tc	1149.37	K	Joback Method

Sources

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=U321947&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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