Isophthalic acid, monoamide, N-(2-ethylhexyl)-, pentyl ester

Inchi: InChI=1S/C21H33NO3/c1-4-7-9-14-25-21(24)19-13-10-12-18(15-19)20(23)22-16-17(6-3)

InchiKey: TXRLEXHCUIISOB-UHFFFAOYSA-N

Formula: C21H33NO3

SMILES: CCCCCOC(=O)c1cccc(C(O)=NCC(CC)CCCC)c1

Mol. weight [g/mol]: 347.49

Physical Properties

Property code	Value	Unit	Source
hf	-581.59	kJ/mol	Joback Method
hvap	94.12	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.555		Crippen Method
mcvol	301.980	ml/mol	McGowan Method
pc	1212.36	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
tb	956.13	K	Joback Method
tc	1171.56	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345837&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