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

Inchi: InChI=1S/C22H35NO3/c1-5-7-11-18(6-2)16-23-21(24)19-12-8-13-20(15-19)22(25)26-14-

InchiKey: AMNCMIOTLHVHSW-UHFFFAOYSA-N

Formula: C22H35NO3

SMILES: CCCCC(CC)CN=C(O)c1cccc(C(=O)OCCCC(C)C)c1

Mol. weight [g/mol]: 361.52

Physical Properties

Property code	Value	Unit	Source
hf	-607.51	kJ/mol	Joback Method
hvap	95.96	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.801		Crippen Method
mcvol	316.070	ml/mol	McGowan Method
pc	1141.34	kPa	Joback Method
rinpol	2853.00		NIST Webbook
rinpol	2853.00		NIST Webbook
tb	978.57	K	Joback Method
tc	1198.36	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345838&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature