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

Inchi: InChI=1S/C22H35NO3/c1-4-7-9-10-15-26-22(25)20-14-11-13-19(16-20)21(24)23-17-18(6

InchiKey: MYRZZNBEOUZXJV-UHFFFAOYSA-N

Formula: C22H35NO3

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

Mol. weight [g/mol]: 361.52

Physical Properties

Property code	Value	Unit	Source
hf	-602.23	kJ/mol	Joback Method
hvap	96.34	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.945		Crippen Method
mcvol	316.070	ml/mol	McGowan Method
pc	1135.20	kPa	Joback Method
rinpol	2903.00		NIST Webbook
rinpol	2903.00		NIST Webbook
tb	979.01	K	Joback Method
tc	1198.66	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345839&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