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

Inchi: InChI=1S/C25H41NO3/c1-4-7-9-10-11-12-13-18-29-25(28)23-17-14-16-22(19-23)24(27)2

InchiKey: GELHSZURGOKUJM-UHFFFAOYSA-N

Formula: C25H41NO3

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

Mol. weight [g/mol]: 403.60

Physical Properties

Property code	Value	Unit	Source
hf	-664.15	kJ/mol	Joback Method
hvap	103.02	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	7.115		Crippen Method
mcvol	358.340	ml/mol	McGowan Method
pc	943.26	kPa	Joback Method
rinpol	3225.00		NIST Webbook
rinpol	3225.00		NIST Webbook
tb	1047.65	K	Joback Method
tc	1286.46	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345842&Units=SI

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