Isophthalic acid, monoamide, N-(3-methylphenyl)-, isohexyl ester

Inchi: InChI=1S/C21H25NO3/c1-15(2)7-6-12-25-21(24)18-10-5-9-17(14-18)20(23)22-19-11-4-8

InchiKey: XXIAEXWYUDCZAS-UHFFFAOYSA-N

Formula: C21H25NO3

SMILES: Cc1cccc(N=C(O)c2cccc(C(=O)OCCCC(C)C)c2)c1

Mol. weight [g/mol]: 339.43

Physical Properties

Property code	Value	Unit	Source
hf	-356.53	kJ/mol	Joback Method
hvap	97.06	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.224		Crippen Method
mcvol	278.220	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinpol	3027.00		NIST Webbook
rinpol	3027.00		NIST Webbook
tb	987.79	K	Joback Method
tc	1218.45	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=U345790&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