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

Inchi: InChI=1S/C20H23NO3/c1-3-4-5-12-24-20(23)17-10-7-9-16(14-17)19(22)21-18-11-6-8-15

InchiKey: HHUAMJHWANZNIZ-UHFFFAOYSA-N

Formula: C20H23NO3

SMILES: CCCCCOC(=O)c1cccc(C(O)=Nc2cccc(C)c2)c1

Mol. weight [g/mol]: 325.40

Physical Properties

Property code	Value	Unit	Source
hf	-330.61	kJ/mol	Joback Method
hvap	95.22	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.978		Crippen Method
mcvol	264.130	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	2969.00		NIST Webbook
rinpol	2969.00		NIST Webbook
tb	965.35	K	Joback Method
tc	1193.64	K	Joback Method

Sources

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=U345789&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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