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

Inchi: InChI=1S/C19H21NO3/c1-13(2)12-23-19(22)16-8-5-7-15(11-16)18(21)20-17-9-4-6-14(3)
InchiKey: OJYCLADVRIHJAK-UHFFFAOYSA-N
Formula: C19H21NO3
SMILES: Cc1cccc(N=C(O)c2cccc(C(=O)OCC(C)C)c2)c1
Mol. weight [g/mol]: 311.37

Physical Properties

Property code	Value	Unit	Source
hf	-315.25	kJ/mol	Joback Method
hvap	92.60	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.444		Crippen Method
mcvol	250.040	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	2797.00		NIST Webbook
rinpol	2797.00		NIST Webbook
tb	942.03	K	Joback Method
tc	1172.63	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=U345787&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