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

Inchi: InChI=1S/C19H21NO3/c1-3-4-11-23-19(22)16-9-6-8-15(13-16)18(21)20-17-10-5-7-14(2)
InchiKey: SLFOTELQRXSPKH-UHFFFAOYSA-N
Formula: C19H21NO3
SMILES: CCCCOC(=O)c1cccc(C(O)=Nc2cccc(C)c2)c1
Mol. weight [g/mol]: 311.37

Physical Properties

Property code	Value	Unit	Source
hf	-309.97	kJ/mol	Joback Method
hvap	92.99	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.588		Crippen Method
mcvol	250.040	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinpol	2852.00		NIST Webbook
rinpol	2852.00		NIST Webbook
tb	942.47	K	Joback Method
tc	1170.78	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345788&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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