

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

Inchi:	InChI=1S/C21H25NO3/c1-3-4-5-6-13-25-21(24)18-11-8-10-17(15-18)20(23)22-19-12-7-9
InchiKey:	MCSACYHHGVATTE-UHFFFAOYSA-N
Formula:	C21H25NO3
SMILES:	CCCCCOC(=O)c1cccc(C(O)=Nc2cccc(C)c2)c1
Mol. weight [g/mol]:	339.43

Physical Properties

Property code	Value	Unit	Source
hf	-351.25	kJ/mol	Joback Method
hvap	97.44	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.368		Crippen Method
mcvol	278.220	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
rinpol	3079.00		NIST Webbook
rinpol	3079.00		NIST Webbook
tb	988.23	K	Joback Method
tc	1217.36	K	Joback Method

Sources

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=U345791&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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