

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

Inchi:	InChI=1S/C18H19NO3/c1-3-10-22-18(21)15-8-5-7-14(12-15)17(20)19-16-9-4-6-13(2)11-
InchiKey:	IOBHQTOILXZSKW-UHFFFAOYSA-N
Formula:	C18H19NO3
SMILES:	CCCOC(=O)c1cccc(C(O)=Nc2cccc(C)c2)c1
Mol. weight [g/mol]:	297.35

Physical Properties

Property code	Value	Unit	Source
hf	-289.33	kJ/mol	Joback Method
hvap	90.77	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.198		Crippen Method
mcvol	235.950	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook
tb	919.59	K	Joback Method
tc	1148.73	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=U345786&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

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