

Nicotinamide, N-(2-iodo-4-methylphenyl)-

Inchi:	InChI=1S/C13H11IN2O/c1-9-4-5-12(11(14)7-9)16-13(17)10-3-2-6-15-8-10/h2-8H,1H3,(H
InchiKey:	MYXYMRYJDVXNLX-UHFFFAOYSA-N
Formula:	C13H11IN2O
SMILES:	Cc1ccc(NC(=O)c2cccnc2)c(I)c1
Mol. weight [g/mol]:	338.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Crippen Method
logp	3.247		Crippen Method
mcvol	193.860	ml/mol	McGowan Method
rinpol	2489.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308110&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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