

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

Inchi:	InChI=1S/C13H11IN2O/c1-9-2-3-12(11(14)8-9)16-13(17)10-4-6-15-7-5-10/h2-8H,1H3,(H
InchiKey:	YQWDRXLDBSNTLV-UHFFFAOYSA-N
Formula:	C13H11IN2O
SMILES:	Cc1ccc(NC(=O)c2ccncc2)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
rinpole	2452.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307417&Units=SI

Legend

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

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<https://www.chemeo.com/cid/15-323-6/Isonicotinamide-N-2-iodo-4-methylphenyl.pdf>

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