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]: 338.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Cheméo Relay (1.0)
logp	3.247		Crippen Method
mcvol	193.860	ml/mol	McGowan Method
rinpol	2452.00		NIST Webbook
tf	479.09	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307417&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point