

Thiophene-2-carboxamide, N-(2-iodo-4-methylphenyl)-

Inchi: InChI=1S/C12H10INOS/c1-8-4-5-10(9(13)7-8)14-12(15)11-3-2-6-16-11/h2-7H,1H3,(H,14)
InchiKey: MLWWQDRORUDPOF-UHFFFAOYSA-N
Formula: C12H10INOS
SMILES: Cc1ccc(NC(=O)c2cccs2)c(I)c1
Mol. weight [g/mol]: 343.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	3.913		Crippen Method
mcvol	190.440	ml/mol	McGowan Method
rinpola	2458.00		NIST Webbook
rinpola	2458.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307075&Units=SI>

Legend

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

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