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

Inchi: InChI=1S/C12H10INO2/c1-8-4-5-10(9(13)7-8)14-12(15)11-3-2-6-16-11/h2-7H,1H3,(H,14
InchiKey: AXBIGBCGFLXMGK-UHFFFAOYSA-N
Formula: C12H10INO2
SMILES: Cc1ccc(NC(=O)c2ccco2)c(I)c1
Mol. weight [g/mol]: 327.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.81		Crippen Method
logp	3.445		Crippen Method
mcvol	179.960	ml/mol	McGowan Method
rinpol	2212.00		NIST Webbook
rinpol	2212.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U307042&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.