2-Furancarboxamide, N-(4-bromophenyl)-

Inchi: InChI=1S/C11H8BrNO2/c12-8-3-5-9(6-4-8)13-11(14)10-2-1-7-15-10/h1-7H,(H,13,14)
InchiKey: KAMNXJSIJYSCFV-UHFFFAOYSA-N
Formula: C11H8BrNO2
SMILES: O=C(Nc1ccc(Br)cc1)c1ccco1
Mol. weight [g/mol]: 266.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.34		Crippen Method
logp	3.294		Crippen Method
mcvol	157.550	ml/mol	McGowan Method
rinpol	2019.00		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=U307039&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