

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
rinpole	2019.00		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=U307039&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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