2-Furamide, n-benzimidazole-2-yl-

Inchi: InChI=1S/C12H9N3O2/c16-11(10-6-3-7-17-10)15-12-13-8-4-1-2-5-9(8)14-12/h1-7H,(H2,1
InchiKey: ZVRZJITVEDLUKY-UHFFFAOYSA-N
Formula: C12H9N3O2
SMILES: O=C(Nc1nc2ccccc2[nH]1)c1ccco1
Mol. weight [g/mol]: 227.22
CAS: 21694-48-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.97		Crippen Method
logp	1.926		Crippen Method
mcvol	158.940	ml/mol	McGowan Method

Sources

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=C21694484&Units=SI
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