3-Furancarboxamide, 2-methyl-N-phenyl-

Other names: 2-Methyl-N-phenyl-furan-3-carboxamide
2-methyl-3-furanilide
Fenfuram
Inchi: InChI=1S/C12H11NO2/c1-9-11(7-8-15-9)12(14)13-10-5-3-2-4-6-10/h2-8H,1H3,(H,13,14)
InchiKey: JFSPBVWPKOEZCB-UHFFFAOYSA-N
Formula: C12H11NO2
SMILES: Cc1occc1C(=O)Nc1ccccc1
Mol. weight [g/mol]: 201.22
CAS: 24691-80-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.30		Aqueous Solubility Prediction Method
log10ws	-3.30		Estimated Solubility Method
logp	2.840		Crippen Method
mcvol	154.140	ml/mol	McGowan Method
rinpol	1905.00		NIST Webbook
tf	382.65	K	Aqueous Solubility Prediction Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24691803&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point