Fuberidazole

Other names: 1H-Benzimidazole, 2-(2-furanyl)-
2-(2'-Furyl)-benzimidazole
2-(2-Furanyl)-1H-benzimidazole
2-(2-Furyl)Benzimidazole
2-furan-2-yl-1H-benzimidazole
B-33172
BAY 33172
Bayer 33172
Benzimidazole, 2-(2-furyl)-
Fuberidatol
Fuberidazol
Fuberisazol
Fubridazole
Furidazol
Furidazole
NSC 72670
Voronit
Voronite
W Vii/117

Inchi: InChI=1S/C11H8N2O/c1-2-5-9-8(4-1)12-11(13-9)10-6-3-7-14-10/h1-7H,(H,12,13)

InchiKey: UYJUZNLFJAWNEZ-UHFFFAOYSA-N

Formula: C11H8N2O

SMILES: c1coc(-c2nc3ccccc3[nH]2)c1

Mol. weight [g/mol]: 184.19

CAS: 3878-19-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Aqueous Solubility Prediction Method
logp	2.341		Crippen Method
mcvol	133.300	ml/mol	McGowan Method
rinpol	1857.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1857.00		NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3878191&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
rinpol:	Non-polar retention indices