Fluridone

Other names:	1-Methyl-3-phenyl-5-(3-(trifluoromethyl)phenyl)-4-pyridone 1-methyl-3-phenyl-5-[3-(trifluoromethyl)phenyl]pyridin-4-one 4(1H)-Pyridinone, 1-methyl-3-phenyl-5-[3-(trifluoromethyl)phenyl]- Sonar
Inchi:	InChI=1S/C19H14F3NO/c1-23-11-16(13-6-3-2-4-7-13)18(24)17(12-23)14-8-5-9-15(10-14
InchiKey:	YWBVHLJPRPCRSD-UHFFFAOYSA-N
Formula:	C19H14F3NO
SMILES:	Cn1cc(-c2ccccc2)c(=O)c(-c2cccc(C(F)(F)F)c2)c1
Mol. weight [g/mol]:	329.32
CAS:	59756-60-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.44		Aqueous Solubility Prediction Method
log10ws	-4.45		Estimated Solubility Method
logp	4.738		Crippen Method
mcvol	228.450	ml/mol	McGowan Method
rinpol	2903.00		NIST Webbook
tf	427.65	K	Aqueous Solubility Prediction Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59756604&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

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