Flurochloridon

Other names: 3-chloro-4-(chloromethyl)-1-[3-(trifluoromethyl)phenyl]pyrrolidin-2-one
FLUROCHLORIDONE
Fluorochloridone
Inchi: InChI=1S/C12H10Cl2F3NO/c13-5-7-6-18(11(19)10(7)14)9-3-1-2-8(4-9)12(15,16)17/h1-4
InchiKey: OQZCSNDVOWYALR-UHFFFAOYSA-N
Formula: C12H10Cl2F3NO
SMILES: O=C1C(Cl)C(CCl)CN1c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 312.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.05		Aqueous Solubility Prediction Method
log10ws	-4.05		Estimated Solubility Method
logp	3.514		Crippen Method
mcvol	186.660	ml/mol	McGowan Method
tf	340.80	K	Aqueous Solubility Prediction Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61213250&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
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

Legend

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