furosemide

Inchi: InChI=1S/C12H11ClN2O5S/c13-9-5-10(15-6-7-2-1-3-20-7)8(12(16)17)4-11(9)21(14,18)1
InchiKey: ZZUFCTLCJUWOSV-UHFFFAOYSA-N
Formula: C12H11ClN2O5S
SMILES: NS(=O)(=O)c1cc(C(=O)O)c(NCc2ccco2)cc1Cl
Mol. weight [g/mol]: 330.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.78		Aqueous Solubility Prediction Method
log10ws	-4.23		Aqueous Solubility Prediction Method
logp	1.891		Crippen Method
mcvol	210.320	ml/mol	McGowan Method
tf	496.79	K	Aqueous Solubility Prediction Method
tf	496.79	K	Aqueous Solubility Prediction Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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
tf: Normal melting (fusion) point