guanine

Inchi: InChI=1S/C17H19F2N3O3/c1-3-21-8-11(17(24)25)16(23)10-6-12(18)15(13(19)14(10)21)
InchiKey: ZEKZLJVOYLTDKK-UHFFFAOYSA-N
Formula: C17H19F2N3O3
SMILES: CCn1cc(C(=O)O)c(=O)c2cc(F)c(N3CCNC(C)C3)c(F)c21
Mol. weight [g/mol]: 351.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.43		Aqueous Solubility Prediction Method
logp	1.796		Crippen Method
mcvol	243.100	ml/mol	McGowan Method
tf	512.92	K	Aqueous Solubility Prediction Method

Sources

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
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
tf: Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.