3-fluoro-pyridine-1-oxide

Inchi: InChI=1S/C5H4FNO/c6-5-2-1-3-7(8)4-5/h1-4H
InchiKey: QVGBDRDOWKIYHK-UHFFFAOYSA-N
Formula: C5H4FNO
SMILES: [O-][n+]1cccc(F)c1
Mol. weight [g/mol]: 113.09
CAS: 695-37-4

Physical Properties

Property code	Value	Unit	Source
affp	900.10	kJ/mol	NIST Webbook
basg	867.60	kJ/mol	NIST Webbook
log10ws	-3.33		Crippen Method
logp	0.459		Crippen Method
mcvol	75.170	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C695374&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume