4-F-phenoxy

Inchi: InChI=1S/C6H4FO/c7-5-1-3-6(8)4-2-5/h1-4H
InchiKey: QDKWLJJOYIFEBS-UHFFFAOYSA-N
Formula: C6H4FO
SMILES: [O]c1ccc(F)cc1
Mol. weight [g/mol]: 111.09
CAS: 2145-21-3

Physical Properties

Property code	Value	Unit	Source
affp	854.50	kJ/mol	NIST Webbook
basg	822.00	kJ/mol	NIST Webbook
log10ws	-5.98		Crippen Method
logp	1.969		Crippen Method
mcvol	77.130	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=C2145213&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