4-fluoropyrazole

Inchi: InChI=1S/C3H3FN2/c4-3-1-5-6-2-3/h1-2H,(H,5,6)
InchiKey: RYXJXPHWRBWEEB-UHFFFAOYSA-N
Formula: C3H3FN2
SMILES: Fc1cn[nH]c1
Mol. weight [g/mol]: 86.07
CAS: 35277-02-2

Physical Properties

Property code	Value	Unit	Source
affp	863.00	kJ/mol	NIST Webbook
basg	829.40	kJ/mol	NIST Webbook
log10ws	-0.79		Crippen Method
logp	0.067		Crippen Method
mcvol	55.400	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35277022&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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