

Pyrazine,tetrafluoro-

Inchi: InChI=1S/C4F4N2/c5-1-2(6)10-4(8)3(7)9-1
InchiKey: VFTWLRXDHOBEDB-UHFFFAOYSA-N
Formula: C4F4N2
SMILES: Fc1nc(F)c(F)nc1F
Mol. weight [g/mol]: 152.05
CAS: 13177-77-0

Physical Properties

Property code	Value	Unit	Source
ie	10.37	eV	NIST Webbook
ie	10.34	eV	NIST Webbook
log10ws	-2.33		Crippen Method
logp	1.033		Crippen Method
mcvol	70.500	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C13177770&Units=SI>

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/14-388-6/Pyrazine-tetrafluoro.pdf>

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