1H-Pyrazole, 5-methoxy-1,3-dimethyl-

Other names: Pyrazole, 1,3-dimethyl-5-methoxy
Inchi: InChI=1S/C6H10N2O/c1-5-4-6(9-3)8(2)7-5/h4H,1-3H3
InchiKey: QGVNQBGVRVIBMA-UHFFFAOYSA-N
Formula: C6H10N2O
SMILES: COc1cc(C)nn1C
Mol. weight [g/mol]: 126.16
CAS: 53091-80-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	0.737		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
ripol	1103.00		NIST Webbook
ripol	1103.00		NIST Webbook

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=C53091808&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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