1H-Pyrazole, 1,3-dimethyl-

Other names: Pyrazole, 1,3-dimethyl-
1,3-Dimethylpyrazole
2,5-Dimethylpyrazole
Inchi: InChI=1S/C5H8N2/c1-5-3-4-7(2)6-5/h3-4H,1-2H3
InchiKey: NODLZCJDRXTSJO-UHFFFAOYSA-N
Formula: C5H8N2
SMILES: Cc1ccn(C)n1
Mol. weight [g/mol]: 96.13
CAS: 694-48-4

Physical Properties

Property code	Value	Unit	Source
affp	933.90	kJ/mol	NIST Webbook
basg	902.30	kJ/mol	NIST Webbook
log10ws	-3.00		Crippen Method
logp	0.729		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
rinpol	833.00		NIST Webbook
rinpol	833.00		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=C694484&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
rinpol:	Non-polar retention indices