3,4,5-Trimethylpyrazole

Other names: 1H-Pyrazole, 3,4,5-trimethyl-
Inchi: InChI=1S/C6H10N2/c1-4-5(2)7-8-6(4)3/h1-3H3,(H,7,8)
InchiKey: HUVAAOZUPLEYBH-UHFFFAOYSA-N
Formula: C6H10N2
SMILES: Cc1n[nH]c(C)c1C
Mol. weight [g/mol]: 110.16
CAS: 5519-42-6

Physical Properties

Property code	Value	Unit	Source
affp	949.30	kJ/mol	NIST Webbook
basg	916.00	kJ/mol	NIST Webbook
log10ws	-1.88		Crippen Method
logp	0.853		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
ripol	2194.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5519426&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

ripol: Polar retention indices