1,5-dimethyl-2(1H)-pyrazinone

Inchi: InChI=1S/C6H8N2O/c1-5-4-8(2)6(9)3-7-5/h3-4H,1-2H3
InchiKey: AEYNPCBTXZXDNL-UHFFFAOYSA-N
Formula: C6H8N2O
SMILES: Cc1cn(C)c(=O)cn1
Mol. weight [g/mol]: 124.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.42		Crippen Method
logp	0.089		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
rinpol	1379.00		NIST Webbook
rinpol	1379.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R221035&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

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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