1,5,6-trimethyl-2(1H)-pyrazinone

Inchi: InChI=1S/C7H10N2O/c1-5-6(2)9(3)7(10)4-8-5/h4H,1-3H3
InchiKey: FUCUUWDBHGJYML-UHFFFAOYSA-N
Formula: C7H10N2O
SMILES: Cc1ncc(=O)n(C)c1C
Mol. weight [g/mol]: 138.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.90		Crippen Method
logp	0.397		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R221015&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.