3,5,6-trimethyl-2(1H)-pyrazinone

Other names: Trimethylpyrazinone
Inchi: InChI=1S/C7H10N2O/c1-4-5(2)9-7(10)6(3)8-4/h1-3H3,(H,9,10)
InchiKey: XOHWPXVKBZHLQO-UHFFFAOYSA-N
Formula: C7H10N2O
SMILES: Cc1nc(C)c(=O)[nH]c1C
Mol. weight [g/mol]: 138.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.31		Crippen Method
logp	0.213		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
ripol	2410.00		NIST Webbook
ripol	2410.00		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=R292621&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