3,5-dimethyl-6-ethyl-2(1H)-pyrazinone

Inchi: InChI=1S/C8H12N2O/c1-4-7-5(2)9-6(3)8(11)10-7/h4H2,1-3H3,(H,10,11)
InchiKey: OJDOIYRLMJWDGW-UHFFFAOYSA-N
Formula: C8H12N2O
SMILES: CCc1[nH]c(=O)c(C)nc1C
Mol. weight [g/mol]: 152.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.63		Crippen Method
logp	0.467		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
ripol	2445.00		NIST Webbook
ripol	2445.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R299444&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
ripol: Polar retention indices

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