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

Inchi: InChI=1S/C9H14N2O/c1-4-5-8-6(2)11-9(12)7(3)10-8/h4-5H2,1-3H3,(H,11,12)
InchiKey: MFJZTQAXJVNSKX-UHFFFAOYSA-N
Formula: C9H14N2O
SMILES: CCCc1nc(C)c(=O)[nH]c1C
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.05		Crippen Method
logp	0.857		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
ripol	2457.00		NIST Webbook
ripol	2457.00		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=R299479&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

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