

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

Inchi:	InChI=1S/C9H14N2O/c1-4-5-8-6(2)10-7(3)9(12)11-8/h4-5H2,1-3H3,(H,11,12)
InchiKey:	GWLWZLSLEQLJJD-UHFFFAOYSA-N
Formula:	C9H14N2O
SMILES:	CCCc1[nH]c(=O)c(C)nc1C
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	2537.00		NIST Webbook
ripol	2537.00		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=R299459&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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