1,6-dimethyl-3-isobutyl-2(1H)-pyrazinone

Inchi: InChI=1S/C10H16N2O/c1-7(2)5-9-10(13)12(4)8(3)6-11-9/h6-7H,5H2,1-4H3
InchiKey: LTTGQZRCQUXHHB-UHFFFAOYSA-N
Formula: C10H16N2O
SMILES: Cc1cnc(CC(C)C)c(=O)n1C
Mol. weight [g/mol]: 180.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	1.287		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
rinpol	1562.00		NIST Webbook
rinpol	1562.00		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=R221055&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
rinpol: Non-polar retention indices

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