1-methyl-3-isobutyl-2(1H)-pyrazinone

Inchi: InChI=1S/C9H14N2O/c1-7(2)6-8-9(12)11(3)5-4-10-8/h4-5,7H,6H2,1-3H3
InchiKey: TZUVQXWVTMFJMV-UHFFFAOYSA-N
Formula: C9H14N2O
SMILES: CC(C)Cc1nccn(C)c1=O
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.35		Crippen Method
logp	0.979		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
rinpol	1397.00		NIST Webbook
rinpol	1397.00		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=R221075&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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