1,5,6-trimethyl-3-isobutyl-2(1H)-pyrazinone

Inchi: InChI=1S/C11H18N2O/c1-7(2)6-10-11(14)13(5)9(4)8(3)12-10/h7H,6H2,1-5H3
InchiKey: RILXBJSXFPLPKB-UHFFFAOYSA-N
Formula: C11H18N2O
SMILES: Cc1nc(CC(C)C)c(=O)n(C)c1C
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.30		Crippen Method
logp	1.596		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
rinpol	1638.00		NIST Webbook
rinpol	1638.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R221020&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.