

Pyrazinecarboxamide, 3,4-dihydro-3-oxo-

Other names:	Pyrazine-2-carboxamide, 3-hydroxy- 2-Pyrazinecarboxamide, 3-hydroxy-
Inchi:	InChI=1S/C5H5N3O2/c6-4(9)3-5(10)8-2-1-7-3/h1-2H,(H2,6,9)(H,8,10)
InchiKey:	SZPBAPFUXAADQV-UHFFFAOYSA-N
Formula:	C5H5N3O2
SMILES:	NC(=O)c1nccnc1O
Mol. weight [g/mol]:	139.11
CAS:	55321-99-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.72		Crippen Method
logp	-0.719		Crippen Method
mcvol	94.930	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C55321998&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/27-284-7/Pyrazinecarboxamide-3-4-dihydro-3-oxo.pdf>

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