

2-Oxo-1-methyl-3-isopropylpyrazine

Other names:	Pyrazine, 2-oxo-1-methyl-3-(1-methylethyl)
Inchi:	InChI=1S/C8H12N2O/c1-6(2)7-8(11)10(3)5-4-9-7/h4-6H,1-3H3
InchiKey:	DPPMIAOELVJMCJ-UHFFFAOYSA-N
Formula:	C8H12N2O
SMILES:	CC(C)c1nccn(C)c1=O
Mol. weight [g/mol]:	152.19
CAS:	78210-68-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.13		Crippen Method
logp	0.904		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
rinpol	1225.00		NIST Webbook
ripol	2160.00		NIST Webbook
ripol	2160.00		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=C78210681&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
ripol:	Polar retention indices

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