

Acetonylprazine

Other names:	Pyrazine, acetonyl
Inchi:	InChI=1S/C7H8N2O/c1-6(10)4-7-5-8-2-3-9-7/h2-3,5H,4H2,1H3
InchiKey:	HKVMSCXHSSBGRU-UHFFFAOYSA-N
Formula:	C7H8N2O
SMILES:	CC(=O)Cc1cnccn1
Mol. weight [g/mol]:	136.15
CAS:	6784-62-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.50		Crippen Method
logp	0.608		Crippen Method
mcvol	107.260	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=C6784629&Units=SI

Legend

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

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