2-Acetylpyrazine

Other names:	acetylpyrazine
	pyrazine, acetyl-
Inchi:	InChI=1S/C6H6N2O/c1-5(9)6-4-7-2-3-8-6/h2-4H,1H3
InchiKey:	DBZAKQWXICEWNW-UHFFFAOYSA-N
Formula:	C6H6N2O
SMILES:	CC(=O)c1cnccn1
Mol. weight [g/mol]:	122.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	0.679		Crippen Method
mcvol	93.170	ml/mol	McGowan Method
rinpol	1033.00		NIST Webbook
rinpol	1033.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Pyrazine and Its Derivatives in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je0601457
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U109047&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