

Aminopyrazine

Other names:	2-Aminopyrazine Pyrazine amine Pyrazinamine- ENT 60202 Pyrazine, amino- Pyrazine, 1,2-dihydro-2-imino- Pyrazine, 2-amino- 1,2-Dihydro-2-iminopyrazine
Inchi:	InChI=1S/C4H5N3/c5-4-3-6-1-2-7-4/h1-3H,(H2,5,7)
InchiKey:	XFTQRUTUGRCSGO-UHFFFAOYSA-N
Formula:	C4H5N3
SMILES:	Nc1cnccn1
Mol. weight [g/mol]:	95.10
CAS:	5049-61-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.64		Crippen Method
logp	0.059		Crippen Method
mcvol	73.400	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=C5049616&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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