

[1,2,3]Triazolo[1,5-a]pyrazine

Inchi:	InChI=1S/C5H4N4/c1-2-9-5(3-6-1)4-7-8-9/h1-4H
InchiKey:	YAFOJTVLHTUFQV-UHFFFAOYSA-N
Formula:	C5H4N4
SMILES:	c1cn2nncc2cn1
Mol. weight [g/mol]:	120.11
CAS:	51392-75-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.73		Crippen Method
logp	0.124		Crippen Method
mcvol	82.310	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51392757&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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