

Isopropylpyrazine

Other names:	2-isopropylpyrazine
Inchi:	InChI=1S/C7H10N2/c1-6(2)7-5-8-3-4-9-7/h3-6H,1-2H3
InchiKey:	GIMBKDZNMKTZMG-UHFFFAOYSA-N
Formula:	C7H10N2
SMILES:	CC(C)c1cncn1
Mol. weight [g/mol]:	122.17
CAS:	9820-90-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	1.600		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
rinpol	949.00		NIST Webbook
rinpol	949.00		NIST Webbook
ripol	1385.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C9820900&Units=SI
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

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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