

2-Isopropyl-3-methylthiopyrazine

Other names:	Pyrazine, 3-(1-methylethyl)-2-(methylthio) Pyrazine, 2-methylthio-3-(1-methylethyl) 3-Isopropyl-2-(methylthio)pyrazine 2-(1-methylethyl)-3-(methylthio)pyrazine
Inchi:	InChI=1S/C8H12N2S/c1-6(2)7-8(11-3)10-5-4-9-7/h4-6H,1-3H3
InchiKey:	MUSIVZZZFRJWGI-UHFFFAOYSA-N
Formula:	C8H12N2S
SMILES:	CS _c 1nccnc1C(C)C
Mol. weight [g/mol]:	168.26
CAS:	67952-59-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Crippen Method
logp	2.322		Crippen Method
mcvol	136.130	ml/mol	McGowan Method
rinpol	1273.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1273.00		NIST Webbook
ripol	1692.00		NIST Webbook
ripol	1692.00		NIST Webbook
ripol	1692.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67952594&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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