

Pyrazine, (2-methylpropyl)-

Other names:	(2-Methylpropyl)pyrazine 2-Isobutylpyrazine 2-(2-Methylpropyl)pyrazine Isobutylpyrazine
Inchi:	InChI=1S/C8H12N2/c1-7(2)5-8-6-9-3-4-10-8/h3-4,6-7H,5H2,1-2H3
InchiKey:	YAIMUUJMJBXAA-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	CC(C)Cc1cnccn1
Mol. weight [g/mol]:	136.19
CAS:	29460-92-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	1.675		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
rinpol	1043.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1043.00		NIST Webbook
ripol	1465.00		NIST Webbook
ripol	1406.00		NIST Webbook
ripol	1465.00		NIST Webbook
ripol	1406.00		NIST Webbook

Sources

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=C29460922&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
ripol:	Polar retention indices

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