

2-(1-Methylpropyl)pyrazine

Other names:	2-Sec-butylpyrazine 1-Methylpropylpyrazine Pyrazine, (1-methylpropyl) sec-Butylpyrazine
Inchi:	InChI=1S/C8H12N2/c1-3-7(2)8-6-9-4-5-10-8/h4-7H,3H2,1-2H3
InchiKey:	NFFQZEXYZVZKNN-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	CCC(C)c1cncn1
Mol. weight [g/mol]:	136.19
CAS:	29460-93-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	1.990		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
rinpol	1040.00		NIST Webbook
rinpol	1040.00		NIST Webbook
ripol	1479.00		NIST Webbook
ripol	1479.00		NIST Webbook
ripol	1479.00		NIST Webbook

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=C29460933&Units=SI

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

Latest version available from:

<https://www.cheméo.com/cid/22-644-2/2-1-Methylpropyl-pyrazine.pdf>

Generated by Cheméo on 2024-04-20 08:41:55.761280834 +0000 UTC m=+15891764.681858149.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.