

Pyrazine, 2-methyl-6-propyl-

Other names:	2-Methyl-6-propylpyrazine 6-Methyl-2-propylpyrazine
Inchi:	InChI=1S/C8H12N2/c1-3-4-8-6-9-5-7(2)10-8/h5-6H,3-4H2,1-2H3
InchiKey:	RMVVGACFOGJRMQ-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	CCc1cncc(C)n1
Mol. weight [g/mol]:	136.19
CAS:	29444-46-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	1.738		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
rinpol	1090.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1090.00		NIST Webbook
ripol	1464.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C29444460&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

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