

2-(1-Ethylpropyl)pyrazine

Other names:	Pyrazine, (1-ethylpropyl)- (1-Ethylpropyl)pyrazine
Inchi:	InChI=1S/C9H14N2/c1-3-8(4-2)9-7-10-5-6-11-9/h5-8H,3-4H2,1-2H3
InchiKey:	RMRVGSBHOQLIOB-UHFFFAOYSA-N
Formula:	C9H14N2
SMILES:	CCC(CC)c1cnccn1
Mol. weight [g/mol]:	150.22
CAS:	40790-26-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.03		Crippen Method
logp	2.380		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1121.00		NIST Webbook
ripol	1449.00		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=C40790269&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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