

2-propenylpyrazine

Other names: 2-prop-2-enylpyrazine
Inchi: InChI=1S/C7H8N2/c1-2-3-7-6-8-4-5-9-7/h2,4-6H,1,3H2
InchiKey: NQRKCUVPFJKKOJ-UHFFFAOYSA-N
Formula: C7H8N2
SMILES: C=CCc1ncncc1
Mol. weight [g/mol]: 120.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.08		Crippen Method
logp	1.205		Crippen Method
mcvol	101.390	ml/mol	McGowan Method
rinpola	1043.00		NIST Webbook
ripola	1546.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R225908&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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
rinpola: Non-polar retention indices
ripola: Polar retention indices

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