2-Methyl-3-trans-propenylpyrazine

Inchi: InChI=1S/C8H10N2/c1-3-4-8-7(2)9-5-6-10-8/h3-6H,1-2H3/b4-3+
InchiKey: ZCGRXTTWRNXLQZ-ONEGZZNKSA-N
Formula: C8H10N2
SMILES: CC=Cc1nccnc1C
Mol. weight [g/mol]: 134.18
CAS: 115610-67-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Crippen Method
logp	1.818		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
ripol	1636.00		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=C115610678&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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