(1-propenyl)pyrazine (Z)

Inchi: InChI=1S/C7H8N2/c1-2-3-7-6-8-4-5-9-7/h2-6H,1H3/b3-2-
InchiKey: ZBHYPERRXYKXGT-IHWYPQMZSA-N
Formula: C7H8N2
SMILES: CC=Cc1cnccn1
Mol. weight [g/mol]: 120.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	1.510		Crippen Method
mcvol	101.390	ml/mol	McGowan Method
rinpol	1073.00		NIST Webbook

Sources

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=R227677&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices