5-ethenyl-2-methoxypyrazine

Inchi:	InChI=1S/C7H8N2O/c1-3-6-4-9-7(10-2)5-8-6/h3-5H,1H2,2H3
InchiKey:	TXBHQOLIYRIEKT-UHFFFAOYSA-N
Formula:	C7H8N2O
SMILES:	C=Cc1cnc(OC)cn1
Mol. weight [g/mol]:	136.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.95		Crippen Method
logp	1.128		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
rinpol	1072.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U365947&Units=SI
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

Legend

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

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