3-ethenyl-2-ethoxypyrazine

Inchi: InChI=1S/C8H10N2O/c1-3-7-8(11-4-2)10-6-5-9-7/h3,5-6H,1,4H2,2H3
InchiKey: SHPUHGKVDFEHKJ-UHFFFAOYSA-N
Formula: C8H10N2O
SMILES: C=Cc1nccnc1OCC
Mol. weight [g/mol]: 150.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.36		Crippen Method
logp	1.518		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
rinpol	1132.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U365948&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
rinpol: Non-polar retention indices