2-ethenyl-3,5-dimethylpyrazine

Other names: Pyrazine, 2-ethenyl-3,5-dimethyl
Inchi: InChI=1S/C8H10N2/c1-4-8-7(3)10-6(2)5-9-8/h4-5H,1H2,2-3H3
InchiKey: ZUOLEJGELMNGPM-UHFFFAOYSA-N
Formula: C8H10N2
SMILES: C=Cc1ncc(C)nc1C
Mol. weight [g/mol]: 134.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.78		Crippen Method
logp	1.736		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
rinpol	1102.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1078.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1551.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1553.00		NIST Webbook
ripol	1524.00		NIST Webbook
ripol	1551.00		NIST Webbook
ripol	1552.00		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=R235846&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
ripol:	Polar retention indices