2-Vinyl-5-methylfuran

Other names: 5-methyl-2-vinylfuran
2-Vinyl-5-methyl furane
Inchi: InChI=1S/C7H8O/c1-3-7-5-4-6(2)8-7/h3-5H,1H2,2H3
InchiKey: LTQOQNQWJBSGPF-UHFFFAOYSA-N
Formula: C7H8O
SMILES: C=Cc1ccc(C)o1
Mol. weight [g/mol]: 108.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.50		Crippen Method
logp	2.231		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
rinpol	826.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	815.00		NIST Webbook
ripol	1160.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1152.00		NIST Webbook
ripol	1160.00		NIST Webbook
ripol	1160.00		NIST Webbook
ripol	1154.00		NIST Webbook
ripol	1149.00		NIST Webbook
ripol	1160.00		NIST Webbook
ripol	1134.00		NIST Webbook
ripol	1132.00		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=C10504139&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