5-methyl-2(E)-propenylfuran

Other names: 5-methyl-2-propenylfuran, trans
trans-2-methyl-5n-propenylfuran
Inchi: InChI=1S/C8H10O/c1-3-4-8-6-5-7(2)9-8/h3-6H,1-2H3/b4-3+
InchiKey: QXSXKNKKQRKGJB-ONEGZZNKSA-N
Formula: C8H10O
SMILES: CC=Cc1ccc(C)o1
Mol. weight [g/mol]: 122.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.92		Crippen Method
logp	2.621		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
ripol	1257.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1304.00		NIST Webbook
ripol	1257.00		NIST Webbook
ripol	1304.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1267.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R316455&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
ripol:	Polar retention indices