

Rose furan

Other names:	2-(3-methyl-2-butenyl)-3-methylfuran 2-(3'-methyl-2'-butenyl)-3-methylfuran
Inchi:	InChI=1S/C10H14O/c1-8(2)4-5-10-9(3)6-7-11-10/h4,6-7H,5H2,1-3H3
InchiKey:	UTSGPHXOHJSDBC-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	<chem>CC(C)=CCc1occc1C</chem>
Mol. weight [g/mol]:	150.22
CAS:	15186-51-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.59		Crippen Method
logp	3.097		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1090.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1104.30		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1065.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1415.00		NIST Webbook
ripol	1413.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1415.00		NIST Webbook
ripol	1412.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=C15186513&Units=SI>

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

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