

cis-2-(2-Pentenyl)furan

Other names:	2-[(2Z)-2-Pentenyl]furan (Z)-2-(2-Pentenyl)furan
Inchi:	InChI=1S/C9H12O/c1-2-3-4-6-9-7-5-8-10-9/h3-5,7-8H,2,6H2,1H3/b4-3-
InchiKey:	KQMWMXVDLIDHGY-ARJAWSKDSA-N
Formula:	C9H12O
SMILES:	CCC=CCc1ccco1
Mol. weight [g/mol]:	136.19
CAS:	70424-13-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	2.788		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
rinpol	1002.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1004.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C70424134&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

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