trans-2-(2-Pentenyl)furan

Other names:	2-[(2E)-2-Pentenyl]furan
	2-(Pent-2(E)-enyl)furan
	(E)-2-(2-Pentenyl)furan
	2(trans-2-Pentenyl)furan
	(E)-2-pentenylfuran
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-ONEGZZNKSA-N
Formula:	C9H12O
SMILES:	CCC=CCc1ccco1
Mol. weight [g/mol]:	136.19
CAS:	70424-14-5

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	1001.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	983.60		NIST Webbook
rinpol	1003.50		NIST Webbook
rinpol	983.60		NIST Webbook
rinpol	983.60		NIST Webbook
ripol	1282.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70424145&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices