

Furan, 3-(4-methyl-3-pentenyl)-

Other names:	Perillen Perillene 3-(4-Methyl-3-pentenyl)-furan 3-(4-Methyl-3-pentenyl)-furan (perillene)
Inchi:	InChI=1S/C10H14O/c1-9(2)4-3-5-10-6-7-11-8-10/h4,6-8H,3,5H2,1-2H3
InchiKey:	XNGKCOFXDHYSGR-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CC(C)=CCc1ccoc1
Mol. weight [g/mol]:	150.22
CAS:	539-52-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.54		Crippen Method
logp	3.178		Crippen Method
mcpol	133.870	ml/mol	McGowan Method
rinpol	1086.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1102.10		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1101.00		NIST Webbook

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rinpol	1100.00	NIST Webbook
rinpol	1119.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1101.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1104.00	NIST Webbook
rinpol	1114.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1114.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1102.00	NIST Webbook
rinpol	1126.00	NIST Webbook
rinpol	1101.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1102.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1115.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1102.10	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1109.00	NIST Webbook
ripol	1421.00	NIST Webbook
ripol	1429.00	NIST Webbook
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ripol	1429.00	NIST Webbook
ripol	1429.00	NIST Webbook
ripol	1410.00	NIST Webbook
ripol	1431.00	NIST Webbook
ripol	1405.00	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=C539526&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Non-polar retention indices
ripol:	Polar retention indices

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