

Benzofuran, 6-ethenyl-4,5,6,7-tetrahydro-3,6-dimethyl-5-isopropyl- trans-

Other names:	5-Isopropenyl-3,6-dimethyl-6-vinyl-4,5,6,7-tetrahydro-1-benzofuran, trans- Curzerene Isogermafurene isofuranogermacrene
Inchi:	InChI=1S/C15H20O/c1-6-15(5)8-14-12(11(4)9-16-14)7-13(15)10(2)3/h6,9,13H,1-2,7-8H2
InchiKey:	HICAMHOOTMOHPA-DZGCQCCKSA-N
Formula:	C15H20O
SMILES:	C=CC1(C)Cc2occ(C)c2CC1C(=C)C
Mol. weight [g/mol]:	216.32
CAS:	17910-09-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.92		Crippen Method
logp	4.071		Crippen Method
mcvol	189.160	ml/mol	McGowan Method
rinpol	1499.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1510.50		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1510.50		NIST Webbook
rinpol	1499.00		NIST Webbook
ripol	1898.00		NIST Webbook
ripol	1885.00		NIST Webbook
ripol	1874.00		NIST Webbook
ripol	1888.00		NIST Webbook

ripol	1888.00	NIST Webbook
ripol	1874.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C17910097&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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