

Furanodiene

Other names:	Furanoelemene (furanodiene)
Inchi:	InChI=1S/C15H20O/c1-11-5-4-6-12(2)9-15-14(8-7-11)13(3)10-16-15/h6-7,10H,4-5,8-9H2
InchiKey:	VMDXHYHOJPKFEK-RZWYOFBOSA-N
Formula:	C15H20O
SMILES:	CC1=CCc2c(C)coc2CC(C)=CCC1
Mol. weight [g/mol]:	216.32
CAS:	19912-61-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.40		Crippen Method
logp	4.359		Crippen Method
mcvol	189.160	ml/mol	McGowan Method
ripol	1886.00		NIST Webbook
ripol	1887.00		NIST Webbook
ripol	1886.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19912619&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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