

1,6-methano[10]annulen-11-one

Other names:	Bicyclo[4.4.1]undeca-1,3,5,7,9-pentaen-11-one
Inchi:	InChI=1S/C11H8O/c12-11-9-5-1-2-6-10(11)8-4-3-7-9/h1-8H
InchiKey:	WUJSPQKZDGCKIZ-UHFFFAOYSA-N
Formula:	C11H8O
SMILES:	O=c1c2ccccc1cccc2
Mol. weight [g/mol]:	156.18
CAS:	36628-80-5

Physical Properties

Property code	Value	Unit	Source
ie	8.00	eV	NIST Webbook
ie	8.47	eV	NIST Webbook
log10ws	-2.70		Crippen Method
logp	2.200		Crippen Method
mcvol	124.200	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C36628805&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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