

Dodecamethyl-[6]pericyclyne

Inchi:	InChI=1S/C30H36/c1-25(2)13-15-26(3,4)17-19-28(7,8)21-23-30(11,12)24-22-29(9,10)20
InchiKey:	BRJNVSWZHFRAQA-UHFFFAOYSA-N
Formula:	C30H36
SMILES:	CC1(C)C#CC(C)(C)C#CC(C)(C)C#CC(C)(C)C#CC(C)(C)C#CC(C)(C)C#CC(C)(C)C#C1
Mol. weight [g/mol]:	396.61
CAS:	98127-90-3

Physical Properties

Property code	Value	Unit	Source
ie	8.70	eV	NIST Webbook
ie	9.05	eV	NIST Webbook
log10ws	-9.59		Crippen Method
logp	6.178		Crippen Method
mcvol	371.100	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98127903&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/65-652-6/Dodecamethyl-6-pericyclyne.pdf>

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