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#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