Decamethyl-[5]pericyclyne

Inchi: InChI=1S/C25H30/c1-21(2)11-13-22(3,4)15-17-24(7,8)19-20-25(9,10)18-16-23(5,6)14-12
InchiKey: QOIXDYKIHPKUIQ-UHFFFAOYSA-N
Formula: C25H30
SMILES: CC1(C)C#CC(C)(C)C#CC(C)(C)C#CC(C)(C)C#CC(C)(C)C#C1
Mol. weight [g/mol]: 330.51
CAS: 88057-40-3

Physical Properties

Property code	Value	Unit	Source
ie	8.60	eV	NIST Webbook
log10ws	-7.95		Crippen Method
logp	5.148		Crippen Method
mcvol	309.250	ml/mol	McGowan Method

Sources

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=C88057403&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.