1,5,9-Cyclododecatriyne

Inchi: InChI=1S/C12H12/c1-2-4-6-8-10-12-11-9-7-5-3-1/h1-2,7-10H2
InchiKey: PYXWKTZVNXGDJK-UHFFFAOYSA-N
Formula: C12H12
SMILES: C1#CCCC#CCCC#CCC1
Mol. weight [g/mol]: 156.22
CAS: 60323-50-4

Physical Properties

Property code	Value	Unit	Source
ie	9.00	eV	NIST Webbook
ie	9.24	eV	NIST Webbook
log10ws	-4.12		Crippen Method
logp	2.351		Crippen Method
mcvol	143.280	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=C60323504&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