Meso 1,2,6,7-cyclodecatetraene

Inchi: InChI=1S/C14H20/c1-11-5-6-13(3)10-14(4)8-7-12(2)9-11/h5-8H2,1-4H3
InchiKey: FUNBFLPBNMGKOJ-UHFFFAOYSA-N
Formula: C10H12
SMILES: CC1=C=C(C)CCC(C)=C=C(C)CC1
Mol. weight [g/mol]: 132.20
CAS: 30154-99-5

Physical Properties

Property code	Value	Unit	Source
hf	360.00	kJ/mol	NIST Webbook
log10ws	-5.03		Crippen Method
logp	4.543		Crippen Method
mcvol	180.060	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C30154995&Units=SI
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

Legend

hf: Enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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