1H-Indeno[6,7,1-mna]anthracene

Inchi: InChI=1S/C19H12/c1-2-4-16-14(3-1)11-15-8-7-12-5-6-13-9-10-17(16)19(15)18(12)13/h1-
InchiKey: BYPYPHWWHJIUHH-UHFFFAOYSA-N
Formula: C19H12
SMILES: C1=c2ccc3cc4ccccc4c4ccc(c2c34)C1
Mol. weight [g/mol]: 240.30
CAS: 190-12-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.60		Crippen Method
logp	4.202		Crippen Method
mcvol	185.570	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=C190125&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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