

Benz[de]indeno[2,1-b]anthracene

Inchi: InChI=1S/C24H14/c1-3-8-19-15(6-1)12-18-14-17-13-16-7-2-4-9-20(16)23(17)22-11-5-10
InchiKey: JYZGYESZNFCYFQ-UHFFFAOYSA-N
Formula: C24H14
SMILES: C1=c2ccccc2=c2c1cc1cc3ccccc3c3cccc2c13
Mol. weight [g/mol]: 302.37
CAS: 32881-40-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.41		Crippen Method
logp	5.294		Crippen Method
mcvol	232.260	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=C32881406&Units=SI>

Legend

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

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