

as-Indaceno[2,3-a]phenanthrene

Inchi: InChI=1S/C24H14/c1-2-6-17-15(4-1)8-10-20-19(17)12-13-22-21-11-9-16-5-3-7-18(16)23
InchiKey: UHMCKWZXPVVXCN-UHFFFAOYSA-N
Formula: C24H14
SMILES: C1=Cc2ccc3c(c2=C1)=Cc1c-3ccc2c1ccc1ccccc12
Mol. weight [g/mol]: 302.37
CAS: 24976-60-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.82		Crippen Method
logp	4.609		Crippen Method
mcvol	232.260	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C24976601&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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