

Cyclopent[*i*]indeno[5,6-*a*]anthracene

Inchi:	InChI=1S/C24H14/c1-4-16-10-21-12-20-8-7-19-9-15-3-2-6-18(15)13-23(19)24(20)14-22(
InchiKey:	RBRBOAXISQXHAF-UHFFFAOYSA-N
Formula:	C24H14
SMILES:	C1=Cc2cc3cc4c(ccc5cc6c(cc54)C=CC=6)cc3cc2=C1
Mol. weight [g/mol]:	302.37
CAS:	222-88-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.78		Crippen Method
logp	4.761		Crippen Method
mcvol	232.260	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C222888&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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