

Cyclopent[b]indeno[4,5-g]phenanthrene

Inchi:	InChI=1S/C24H14/c1-3-16-11-20-9-7-15-8-10-21-12-17-4-2-6-19(17)14-23(21)24(15)22(16)
InchiKey:	PFBAAKICFFFAPX-UHFFFAOYSA-N
Formula:	C24H14
SMILES:	<chem>C1=Cc2cc3c(ccc4ccc5cc6c(cc5c43)=CC=C6)cc2=C1</chem>
Mol. weight [g/mol]:	302.37
CAS:	72088-81-4

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72088814&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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