

Dicyclopenta[a,c]naphthacene

Inchi:	InChI=1S/C24H14/c1-2-6-16-12-18-14-24-22-10-4-8-20(22)19-7-3-9-21(19)23(24)13-17(
InchiKey:	PUCMMVRHLCLFFD-UHFFFAOYSA-N
Formula:	C24H14
SMILES:	C1=Cc2c3c(c4cc5cc6ccccc6cc5cc4c2=C1)=CC=C3
Mol. weight [g/mol]:	302.37
CAS:	15209-78-6

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15209786&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/72-370-1/Dicyclopenta-a-c-naphthacene.pdf>

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