

Benz[5,6]indeno[2,1-a]phenalene

Inchi:	InChI=1S/C24H14/c1-2-6-17-12-21-19(11-16(17)5-1)14-22-20-10-4-8-15-7-3-9-18(24(15)
InchiKey:	KXAYQKOGXBEXSV-UHFFFAOYSA-N
Formula:	C24H14
SMILES:	C1=c2c(cc3cccc4cccc2c43)-c2cc3cccc3cc21
Mol. weight [g/mol]:	302.37
CAS:	76727-41-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.89		Crippen Method
logp	5.674		Crippen Method
mcvol	232.260	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76727418&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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