

Benz[c]indeno[2,1-a]fluorene

Inchi:	InChI=1S/C24H14/c1-3-9-17-15(7-1)13-21-22-14-16-8-2-4-10-18(16)24(22)20-12-6-5-11
InchiKey:	ZBDZXWFDPTVMAV-UHFFFAOYSA-N
Formula:	C24H14
SMILES:	C1=c2c(c3ccccc3c3c2=Cc2ccccc2-3)-c2ccccc21
Mol. weight [g/mol]:	302.37
CAS:	201-72-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.87		Crippen Method
logp	4.458		Crippen Method
mcvol	232.260	ml/mol	McGowan Method

Sources

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=C201729&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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