Galathan, 1,2,3,12,15,16-hexadehydro-9,10-[methylenebis(ox

Other names: 5,7-dihydro-4H-[1,3]Dioxolo[4,5-j]pyrrolo[3,2,1-de]phenanthridine
Inchi: InChI=1S/C16H13NO2/c1-2-10-4-5-17-8-11-6-14-15(19-9-18-14)7-13(11)12(3-1)16(10)1
InchiKey: NWJBCDNATQJZOD-UHFFFAOYSA-N
Formula: C16H13NO2
SMILES: c1cc2c3c(c1)-c1cc4c(cc1CN3CC2)OCO4
Mol. weight [g/mol]: 251.28
CAS: 641-89-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	2.958		Crippen Method
mcvol	177.920	ml/mol	McGowan Method
rinpol	2499.00		NIST Webbook
rinpol	2499.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C641894&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol: Non-polar retention indices

Latest version available from: