4-Phenyl-6-chloro-acridone

Inchi: InChI=1S/C19H12ClNO/c20-13-9-10-15-17(11-13)21-18-14(12-5-2-1-3-6-12)7-4-8-16(18
InchiKey: DYCGEGQLXHNSGJ-UHFFFAOYSA-N
Formula: C19H12ClNO
SMILES: O=c1c2ccc(Cl)cc2[nH]c2c(-c3ccccc3)cccc12
Mol. weight [g/mol]: 305.76
CAS: 116345-95-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.01		Crippen Method
logp	4.520		Crippen Method
mcvol	220.220	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116345950&Units=SI

Legend

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