Carbamazepine, M (formyl-acridine)

Inchi: InChI=1S/C15H11NO/c17-11-16-14-7-3-1-5-12(14)9-10-13-6-2-4-8-15(13)16/h1-11H
InchiKey: PFWIZLGRDVDFQK-UHFFFAOYSA-N
Formula: C15H11NO
SMILES: O=CN1c2ccccc2C=Cc2ccccc21
Mol. weight [g/mol]: 221.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	3.465		Crippen Method
mcvol	171.080	ml/mol	McGowan Method
rinpol	2025.00		NIST Webbook

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=R255513&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices