(Z) 9-(2[1-Naphthyl]ethenyl)acridine

Inchi: InChI=1S/C25H17N/c1-2-11-20-18(8-1)9-7-10-19(20)16-17-21-22-12-3-5-14-24(22)26-25
InchiKey: UAHNCBXJWNCMMA-MSUUIHNZSA-N
Formula: C25H17N
SMILES: C(=Cc1c2ccccc2nc2ccccc12)c1cccc2ccccc12
Mol. weight [g/mol]: 331.41
CAS: 134591-96-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.26		Crippen Method
logp	6.712		Crippen Method
mcvol	262.890	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=C134591961&Units=SI

Legend

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