2,5-DIMETHYLPHENYL ACRIDINE-9-CARBOXYLATE

Inchi: InChI=1S/C22H17NO2/c1-14-11-12-15(2)20(13-14)25-22(24)21-16-7-3-5-9-18(16)23-19-

InchiKey: XSOWTYRQEZMPRO-UHFFFAOYSA-N

Formula: C22H17NO2

SMILES: Cc1ccc(C)c(OC(=O)c2c3ccccc3nc3ccccc23)c1

Mol. weight [g/mol]: 327.38

Physical Properties

Property code	Value	Unit	Source
logp	5.224		Crippen Method
mcvol	251.820	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	37.90	kJ/mol	457.00	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C128649376&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfust: Enthalpy of fusion at a given temperature

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume