

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:	<chem>Cc1ccc(C)c(OC(=O)c2c3ccccc3nc3ccccc23)c1</chem>
Mol. weight [g/mol]:	327.38
CAS:	128649-37-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.88		Crippen Method
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

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=C128649376&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hfust: Enthalpy of fusion at a given temperature

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

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