

9-Hydroxy-4-methoxyacridine

Other names:	10H-Acridin-9-one, 4-methoxy-4-Methoxyacridin-9(10H)-one
Inchi:	InChI=1S/C14H11NO2/c1-17-12-8-4-6-10-13(12)15-11-7-3-2-5-9(11)14(10)16/h2-8H,1H3
InchiKey:	ZYEVJRPVZZGDRM-UHFFFAOYSA-N
Formula:	C14H11NO2
SMILES:	COc1cccc2c(=O)c3cccc3[nH]c12
Mol. weight [g/mol]:	225.25

Physical Properties

Property code	Value	Unit	Source
hf	-46.31	kJ/mol	Cheméo Relay (1.0)
ie	7.55	eV	Cheméo Relay (1.0)
logp	2.208		Crippen Method
mcvol	167.160	ml/mol	McGowan Method
tf	500.92	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35308000&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

tf: Normal melting (fusion) point

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