2H-1-BENZOPYRAN-2-ONE, 8-METHOXY-

Other names: Coumarin, 8-methoxy-
Inchi: InChI=1S/C10H8O3/c1-12-8-4-2-3-7-5-6-9(11)13-10(7)8/h2-6H,1H3
InchiKey: ODRDTKMYQDXVGG-UHFFFAOYSA-N
Formula: C10H8O3
SMILES: COc1cccc2ccc(=O)oc12
Mol. weight [g/mol]: 176.17

Physical Properties

Property code	Value	Unit	Source
hf	-291.55	kJ/mol	Cheméo Relay (1.0)
ie	8.36	eV	Cheméo Relay (1.0)
log10ws	-2.37		Cheméo Relay (1.0)
logp	1.802		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
tb	605.86	K	Cheméo Relay (1.0)
tf	362.48	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=C2445810&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf: Enthalpy of formation at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point