COUMARIN-3-CARBOXYLIC ACID

Other names:	2-Oxobenzopyran-3-carboxylic acid
	2-oxo-2H-1-benzopyran-3-carboxylic acid
	2-oxo-2H-chromene-3-carboxylic acid
	2H-1-Benzopyran-3-carboxylic acid, 2-oxo-
	2H-1-benzopyran-2-one-3-carboxylic acid
	3-carboxycoumarin
	Benzopyran-3-carboxylic acid, 2H-1-, 2-oxo
	G 1
	Malonic acid, salicylidene-, «delta»-lactone
Inchi:	InChI=1S/C10H6O4/c11-9(12)7-5-6-3-1-2-4-8(6)14-10(7)13/h1-5H,(H,11,12)
InchiKey:	ACMLKANOGIVEPB-UHFFFAOYSA-N
Formula:	C10H6O4
SMILES:	O=C(O)c1cc2ccccc2oc1=O
Mol. weight [g/mol]:	190.15

Physical Properties

Property code	Value	Unit	Source
hf	-508.52	kJ/mol	Cheméo Relay (1.0)
ie	9.28	eV	Cheméo Relay (1.0)
log10ws	-2.66		Cheméo Relay (1.0)
logp	1.491		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
tb	623.00	K	Cheméo Relay (1.0)
tf	465.57	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Equilibrium partitioning of drug molecules between aqueous and amino acid ester based ionic liquids:	https://www.doi.org/10.1016/j.jct.2013.02.011
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C531817&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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