

2H-Pyran-5-carboxylic acid, 2-oxo-

Other names:	«alpha»-Pyrone-5-carboxylic acid Coumalic acid Cumalic acid 2-Oxopyran-5-carboxylic acid 2-Pentenedioic acid, 4-(hydroxymethylene)-, «delta»-lactone 2-Pyrone-5-carboxylic acid «alpha»-Pyrone-3-carboxylic acid 2-Oxo-1,2H-pyran-5-carboxylic acid
Inchi:	InChI=1S/C6H4O4/c7-5-2-1-4(3-10-5)6(8)9/h1-3H,(H,8,9)
InchiKey:	ORGPJDKNYMVLFL-UHFFFAOYSA-N
Formula:	C6H4O4
SMILES:	O=C(O)c1ccc(=O)oc1
Mol. weight [g/mol]:	140.09
CAS:	500-05-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.69		Crippen Method
logp	0.338		Crippen Method
mcvol	90.820	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	491.20	K	16.00	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=C500050&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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