«alpha»-Furil

Other names:	Ethanedione, di-2-furanyl-
	Furil
	Bipyromucyl
	Difuranylglyoxal
	2,2'-Furil
	Bipryomucyl
	Di-2-furylglyoxal
	Difuroyl
	1,2-Ethanedione, 1,2-di-2-furanyl-
	Di-2-furanylethanedione
	NSC 5561
Inchi:	InChI=1S/C10H6O4/c11-9(7-3-1-5-13-7)10(12)8-4-2-6-14-8/h1-6H
InchiKey:	SXPUVBFQXJHYNS-UHFFFAOYSA-N
Formula:	C10H6O4
SMILES:	O=C(C(=O)c1ccco1)c1ccco1
Mol. weight [g/mol]:	190.15
CAS:	492-94-4

Physical Properties

Property code	Value	Unit	Source
chs	-4453.40	kJ/mol	NIST Webbook
ea	1.34 ± 0.09	eV	NIST Webbook
log10ws	-11.07		Crippen Method
logp	1.938		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
rinpol	1544.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C492944&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
ea:	Electron affinity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices