2,5-Furandicarboxaldehyde

Other names:	5-formylfurfural
	furan-2,5-dicarbaldehyde
	Furan-2,5-dicarboxaldehyde
Inchi:	InChI=1S/C6H4O3/c7-3-5-1-2-6(4-8)9-5/h1-4H
InchiKey:	PXJJKVNIMAZHCB-UHFFFAOYSA-N
Formula:	C6H4O3
SMILES:	O=Cc1ccc(C=O)o1
Mol. weight [g/mol]:	124.09
CAS:	823-82-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	0.905		Crippen Method
mcvol	84.950	ml/mol	McGowan Method
rinpol	1076.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1076.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	1996.00		NIST Webbook
ripol	1991.00		NIST Webbook
ripol	2006.00		NIST Webbook
ripol	1996.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1991.00		NIST Webbook
ripol	1996.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	2006.00		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=C823825&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices