

Furan-2(5H)-one, 3-hydroxy-4,5-dimethyl-

Other names:	Sotolone
	4,5-Dimethyl-3-hydroxy-2(5H)-furanone
	Furan-2(5H)-one, 3-hydroxy-4,5-dimethyl-
	3-Hydroxy-4,5-dimethyl-2(5H)-furanone
	Sotolon
	3-Hydroxy-4,5-dimethyl-5H-furan-2-one
	3-Hydroxy-4,5-dimethylfuran-2(5H)-one
	4,5-Dimethyl-3-hydroxy-2,5-dihydrofuran-2-one
	2,3-Dimethyl-4-hydroxy-2,5-dihydrofuran-5-one
	3-hydroxy-4,5-dimethyl-2(5H)-furanone (sotolon)
	4,5-dimethyl-3-hydroxy-2-(5H)-furanone (sotolon)
	3-hydroxy-4,5-dimethylfuran-2(5H)-one (sotolon)
	4,5-dimethyl-3-hydroxy-2,5-dihydrofuran-2-one (sotolon)
Inchi:	InChI=1S/C6H8O3/c1-3-4(2)9-6(8)5(3)7/h4,7H,1-2H3
InchiKey:	UNYNVICDCJHOPO-UHFFFAOYSA-N
Formula:	C6H8O3
SMILES:	CC1=C(O)C(=O)OC1C
Mol. weight [g/mol]:	128.13

Physical Properties

Property code	Value	Unit	Source
hfus	17.25	kJ/mol	Joback Method
logp	0.764		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
rinpol	1105.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1120.00		NIST Webbook
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rinpol	1113.00		NIST Webbook

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rinpol	1131.00	NIST Webbook
rinpol	1122.00	NIST Webbook
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rinpol	1104.00	NIST Webbook
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ripol	2153.00		NIST Webbook
ripol	2213.00		NIST Webbook
ripol	2214.00		NIST Webbook
ripol	2188.00		NIST Webbook
ripol	2182.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2198.00		NIST Webbook
ripol	2210.00		NIST Webbook
ripol	2186.00		NIST Webbook
ripol	2181.00		NIST Webbook
tf	372.79	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	221.64	J/mol×K	548.03	Joback Method
cpg	231.11	J/mol×K	582.49	Joback Method
cpg	240.20	J/mol×K	616.94	Joback Method
cpg	248.92	J/mol×K	651.40	Joback Method
cpg	257.23	J/mol×K	685.86	Joback Method
cpg	265.12	J/mol×K	720.32	Joback Method
cpg	272.59	J/mol×K	754.77	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C28664359&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point

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