2(5H)-Furanone, 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
CAS:	28664-35-9

Physical Properties

Property code	Value	Unit	Source
gf	-298.64	kJ/mol	Joback Method
hf	-493.78	kJ/mol	Joback Method
hfus	17.25	kJ/mol	Joback Method
hvap	56.26	kJ/mol	Joback Method
log10ws	-0.88		Crippen Method
logp	0.764		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
rinpol	1104.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1111.00		NIST Webbook

rinpol	1107.00	NIST Webbook
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ripol	2210.00		NIST Webbook
ripol	2186.00		NIST Webbook
ripol	2181.00		NIST Webbook
ripol	2182.00		NIST Webbook
tb	548.03	K	Joback Method
tc	754.77	K	Joback Method

tf	349.69	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28664359&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume