Furaneol

Other names:	2,3-Dihydro-4-hydroxy-2,5-dimethyl-3-furanone 2,5-Dimethyl-4(1H)-hydroxy-3(2H)-furanone 2,5-Dimethyl-4-hydroxy-(2H)-furan-3-one 2,5-Dimethyl-4-hydroxy-2,3-dihydrofuran-3-one 2,5-Dimethyl-4-hydroxy-3(2H)-fuiranone 2,5-dimethyl-3-hydroxy-4-oxo-4,5-dihydrofuran 2,5-dimethyl-4,5-dihydrofuran-3-ol-4-one 2,5-dimethyl-4-hydroxy-(2H)-furan-3-one (furaneol) 2,5-dimethyl-4-hydroxy-2,3-dihydrofuran-3-one (furaneol) 2,5-dimethyl-4-hydroxy-3(2H)-furanone 2,5-dimethyl-4-hydroxy-3(2H)-furanone (DMHF) 2,5-dimethyl-4-hydroxy-3(2H)-furanone (Furaneol) 3(2H)-Furanone, 2,5-dimethyl-4-hydroxy- 3(2H)-Furanone, 4-hydroxy-2,5-dimethyl- 4-Hydroxy-2,5-dimethyl-3(2H)furanone 4-Hydroxy-2,5-dimethyl-3-furanone 4-Hydroxy-2,5-dimethylfuran-3(2H)-one 4-hydroxy-2,5-dimethyl-3(2H)-furanone 4-hydroxy-2,5-dimethyl-3(2H)-furanone (Furaneol) 4-hydroxy-2,5-dimethyl-3(2H)-furanone (HDMF) 4-hydroxy-2,5-dimethylfuran-2(3H)-one 4-hydroxy-2,5-dimethylfuran-3(2H)-one (Furaneol) Alletone COE 536 FEMA 3174 Pineapple ketone hydroxy-2,5-dimethyl-3(2H)-4-furanone (Furaneol)
Inchi:	InChI=1S/C6H8O3/c1-3-5(7)6(8)4(2)9-3/h3,8H,1-2H3
InchiKey:	INAXVXBDKKUCGI-UHFFFAOYSA-N
Formula:	C6H8O3
SMILES:	CC1=C(O)C(=O)C(C)O1
Mol. weight [g/mol]:	128.13
CAS:	3658-77-3

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	1065.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1023.00		NIST Webbook
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ripol	2020.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	2028.00		NIST Webbook
tb	548.03	K	Joback Method
tc	754.77	K	Joback Method
tf	353.90	K	Experimental determination and correlation of the solubility of 4-hydroxy-2,5-dimethyl-3(2H)-furanone (DMHF) in six different solvents
tf	355.22	K	Thermodynamic equilibrium of 4-hydroxy-2,5-dimethyl-3(2H)-furanone in different solvent systems

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

Experimental determination and correlation of the solubility of 4-hydroxy-2,5-dimethyl-3(2H)-furanone (DMHF) in six different solvents:	https://www.doi.org/10.1016/j.jct.2015.08.028
Thermodynamic equilibrium of 4-hydroxy-2,5-dimethyl-3(2H)-furanone (DMHF) in different solvent systems:	https://www.doi.org/10.1016/j.jct.2015.08.035
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=C3658773&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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