2,5-Dimethyl-4-hydroxy-2(5H)-furanone

Inchi: InChI=1S/C5H6O3/c1-3-4(6)2-5(7)8-3/h2-3,6H,1H3
InchiKey: JGAAAWQBYJNOIW-UHFFFAOYSA-N
Formula: C5H6O3
SMILES: CC1OC(=O)C=C1O
Mol. weight [g/mol]: 114.10

Physical Properties

Property code	Value	Unit	Source
gf	-297.43	kJ/mol	Joback Method
hf	-461.67	kJ/mol	Joback Method
hfus	15.05	kJ/mol	Joback Method
hvap	53.37	kJ/mol	Joback Method
log10ws	-0.46		Crippen Method
logp	0.374		Crippen Method
mcvol	79.460	ml/mol	McGowan Method
pc	5258.62	kPa	Joback Method
rinpol	1062.00		NIST Webbook
rinpol	1062.00		NIST Webbook
ripol	2024.00		NIST Webbook
ripol	2031.00		NIST Webbook
tb	520.17	K	Joback Method
tc	729.03	K	Joback Method
tf	325.90	K	Joback Method
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.26	J/mol×K	520.17	Joback Method
cpg	188.80	J/mol×K	554.98	Joback Method
cpg	197.00	J/mol×K	589.79	Joback Method
cpg	204.83	J/mol×K	624.60	Joback Method
cpg	212.30	J/mol×K	659.41	Joback Method
cpg	219.39	J/mol×K	694.22	Joback Method

cpg	226.09	J/mol×K	729.03	Joback Method

Sources

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=R516120&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