2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-one

Other names: 2,4-Dihydroxy-2,5-dimethyl-3(2H)-furanone
2,5-Dimethyl-2,4-dihydroxy-3(2H)-furanone
Inchi: InChI=1S/C6H8O4/c1-3-4(7)5(8)6(2,9)10-3/h7,9H,1-2H3
InchiKey: GMQUMWVEWMCMOQ-UHFFFAOYSA-N
Formula: C6H8O4
SMILES: CC1=C(O)C(=O)C(C)(O)O1
Mol. weight [g/mol]: 144.13
CAS: 10230-62-3

Physical Properties

Property code	Value	Unit	Source
gf	-440.95	kJ/mol	Joback Method
hf	-630.77	kJ/mol	Joback Method
hfus	15.04	kJ/mol	Joback Method
hvap	71.79	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	0.084		Crippen Method
mcvol	99.420	ml/mol	McGowan Method
pc	5462.66	kPa	Joback Method
rinpol	1026.80		NIST Webbook
rinpol	1026.80		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	977.00		NIST Webbook
tb	640.45	K	Joback Method
tc	841.00	K	Joback Method
tf	434.41	K	Joback Method
vc	0.362	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.14	J/mol×K	640.45	Joback Method
cpg	267.83	J/mol×K	673.87	Joback Method
cpg	275.26	J/mol×K	707.30	Joback Method

cpg	282.49	J/mol×K	740.72	Joback Method
cpg	289.59	J/mol×K	774.15	Joback Method
cpg	296.60	J/mol×K	807.57	Joback Method
cpg	303.58	J/mol×K	841.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10230623&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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