4-Methyl-5H-furan-2-one

Other names: 4-Methyl-2(5H)-furanone
Inchi: InChI=1S/C5H6O2/c1-4-2-5(6)7-3-4/h2H,3H2,1H3
InchiKey: ZZEYQBNQZKUWKY-UHFFFAOYSA-N
Formula: C5H6O2
SMILES: CC1=CC(=O)OC1
Mol. weight [g/mol]: 98.10
CAS: 6124-79-4

Physical Properties

Property code	Value	Unit	Source
gf	-152.90	kJ/mol	Joback Method
hf	-289.10	kJ/mol	Joback Method
hfus	9.89	kJ/mol	Joback Method
hvap	37.00	kJ/mol	Joback Method
log10ws	-0.53		Crippen Method
logp	0.489		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
pc	4835.95	kPa	Joback Method
ripol	1912.00		NIST Webbook
ripol	1912.00		NIST Webbook
ripol	1909.00		NIST Webbook
tb	432.66	K	Joback Method
tc	656.90	K	Joback Method
tf	269.32	K	Joback Method
vc	0.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.67	J/mol×K	432.66	Joback Method
cpg	149.00	J/mol×K	470.03	Joback Method
cpg	157.97	J/mol×K	507.41	Joback Method
cpg	166.57	J/mol×K	544.78	Joback Method
cpg	174.79	J/mol×K	582.15	Joback Method

cpg	182.62	J/mol×K	619.53	Joback Method
cpg	190.05	J/mol×K	656.90	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=C6124794&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume