5-Methylene-2(5H)-furanone (Protoanemonine)

Inchi: InChI=1S/C5H4O2/c1-4-2-3-5(6)7-4/h2-3H,1H2
InchiKey: RNYZJZKPGHQTJR-UHFFFAOYSA-N
Formula: C5H4O2
SMILES: C=C1C=CC(=O)O1
Mol. weight [g/mol]: 96.08

Physical Properties

Property code	Value	Unit	Source
gf	-90.19	kJ/mol	Joback Method
hf	-193.39	kJ/mol	Joback Method
hfus	9.12	kJ/mol	Joback Method
hvap	36.50	kJ/mol	Joback Method
log10ws	-0.88		Crippen Method
logp	0.613		Crippen Method
mcvol	69.290	ml/mol	McGowan Method
pc	5073.01	kPa	Joback Method
rinpol	880.00		NIST Webbook
rinpol	880.00		NIST Webbook
tb	426.84	K	Joback Method
tc	651.70	K	Joback Method
tf	270.48	K	Joback Method
vc	0.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.70	J/mol×K	426.84	Joback Method
cpg	133.69	J/mol×K	464.32	Joback Method
cpg	141.38	J/mol×K	501.79	Joback Method
cpg	148.75	J/mol×K	539.27	Joback Method
cpg	155.78	J/mol×K	576.75	Joback Method
cpg	162.48	J/mol×K	614.23	Joback Method
cpg	168.83	J/mol×K	651.70	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=R617500&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume