

2(5H)-Furanone, 5-methylene-

Other names:	protoanemonine 5-methylenefuran-2(5H)-one
Inchi:	InChI=1S/C5H4O2/c1-4-2-3-5(6)7-4/h2-3H,1H2
InchiKey:	RNYZJZKPGHQJTR-UHFFFAOYSA-N
Formula:	C5H4O2
SMILES:	C=C1C=CC(=O)O1
Mol. weight [g/mol]:	96.08
CAS:	108-28-1

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	878.00		NIST Webbook
rinpol	878.00		NIST Webbook
ripol	1560.00		NIST Webbook
ripol	1623.00		NIST Webbook
ripol	1623.00		NIST Webbook
ripol	1560.00		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/molxK	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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C108281&Units=SI

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:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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