3(2H)-Furanone

Inchi: InChI=1S/C4H4O2/c5-4-1-2-6-3-4/h1-2H,3H2
InchiKey: LYINKTVZUSKQEQ-UHFFFAOYSA-N
Formula: C4H4O2
SMILES: O=C1C=COC1
Mol. weight [g/mol]: 84.07

Physical Properties

Property code	Value	Unit	Source
gf	-151.69	kJ/mol	Joback Method
hf	-256.99	kJ/mol	Joback Method
hfus	7.69	kJ/mol	Joback Method
hvap	34.11	kJ/mol	Joback Method
log10ws	-0.11		Crippen Method
logp	0.099		Crippen Method
mcvol	59.500	ml/mol	McGowan Method
pc	5678.82	kPa	Joback Method
ripol	1449.00		NIST Webbook
ripol	1449.00		NIST Webbook
tb	404.80	K	Joback Method
tc	630.37	K	Joback Method
tf	245.53	K	Joback Method
vc	0.215	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	103.50	J/mol×K	404.80	Joback Method
cpg	111.68	J/mol×K	442.39	Joback Method
cpg	119.51	J/mol×K	479.99	Joback Method
cpg	126.99	J/mol×K	517.58	Joback Method
cpg	134.12	J/mol×K	555.18	Joback Method
cpg	140.88	J/mol×K	592.77	Joback Method
cpg	147.27	J/mol×K	630.37	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R76171&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:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume