

2(3H)-Furanone, dihydro-4-hydroxy-

Other names:	Dihydro-4-hydroxy-2-(3H)-furanone
Inchi:	InChI=1S/C4H6O3/c5-3-1-4(6)7-2-3/h3,5H,1-2H2
InchiKey:	FUDDLSHBRSNCBV-UHFFFAOYSA-N
Formula:	C4H6O3
SMILES:	O=C1CC(O)CO1
Mol. weight [g/mol]:	102.09
CAS:	5469-16-9

Physical Properties

Property code	Value	Unit	Source
gf	-326.18	kJ/mol	Joback Method
hf	-487.34	kJ/mol	Joback Method
hfus	11.63	kJ/mol	Joback Method
hvap	50.19	kJ/mol	Joback Method
log10ws	0.37		Crippen Method
logp	-0.706		Crippen Method
mcvol	69.670	ml/mol	McGowan Method
pc	5880.91	kPa	Joback Method
rinpol	1185.10		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1185.10		NIST Webbook
rinpol	1153.00		NIST Webbook
ripol	2457.00		NIST Webbook
ripol	2457.00		NIST Webbook
ripol	2457.00		NIST Webbook
tb	493.15	K	Joback Method
tc	701.93	K	Joback Method
tf	301.35	K	Joback Method
vc	0.247	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.21	J/molxK	493.15	Joback Method

cpg	166.07	J/mol×K	527.95	Joback Method
cpg	174.55	J/mol×K	562.74	Joback Method
cpg	182.66	J/mol×K	597.54	Joback Method
cpg	190.39	J/mol×K	632.34	Joback Method
cpg	197.73	J/mol×K	667.13	Joback Method
cpg	204.66	J/mol×K	701.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5469169&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
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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