2(5H)-Furanone, 4-methyl-5-(2-methyl-2-propenyl)-

Inchi: InChI=1S/C9H12O2/c1-6(2)4-8-7(3)5-9(10)11-8/h5,8H,1,4H2,2-3H3
InchiKey: ZATUMQTYNNDDSO-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: C=C(C)CC1OC(=O)C=C1C
Mol. weight [g/mol]: 152.19
CAS: 89902-24-9

Physical Properties

Property code	Value	Unit	Source
gf	-47.64	kJ/mol	Joback Method
hf	-276.36	kJ/mol	Joback Method
hfus	18.73	kJ/mol	Joback Method
hvap	45.01	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.824		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	949.50		NIST Webbook
rinpol	949.50		NIST Webbook
tb	516.07	K	Joback Method
tc	735.62	K	Joback Method
tf	294.44	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.08	J/mol×K	516.07	Joback Method
cpg	301.50	J/mol×K	552.66	Joback Method
cpg	315.23	J/mol×K	589.25	Joback Method
cpg	328.25	J/mol×K	625.84	Joback Method
cpg	340.59	J/mol×K	662.44	Joback Method
cpg	352.24	J/mol×K	699.03	Joback Method
cpg	363.21	J/mol×K	735.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89902249&Units=SI
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

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