2(3H)-Furanone, 5-ethenyldihydro-5-methyl-

Other names: 2(3H)-Furanone, dihydro-5-methyl-5-vinyl-
5-Methyl-5-vinyldihydrofuran-2(3H)-one
«gamma»-Vinyl-«gamma»-valerolactone
4-Methyl-4-vinyl-1,4-butanolide
4-Methyl-4-vinylbutyrolactone
Dihydro-5-methyl-5-vinyl-2(3H)-furanone
5-Hexenoic acid, 4-hydroxy-4-methyl-, «gamma»-lactone
4-Methyl-5-hexen-4-olide
5-Ethenyldihydro-5-methyl-2(3H)-furanone
Lavender lactone
(3H)-Furanone, 5-ethenyldihydro-5-methyl-
«gamma»-Methyl-«gamma»-vinyl-«gamma»-butyrolactone
5-ethenyl-5-methyl-2(3H)-furanone
lavander lactone
dihydro-5-methyl-5-vinylfuran-2(3H)-one

Inchi: InChI=1S/C7H10O2/c1-3-7(2)5-4-6(8)9-7/h3H,1,4-5H2,2H3

InchiKey: QESPSAHXYXIGBG-UHFFFAOYSA-N

Formula: C7H10O2

SMILES: C=CC1(C)CCC(=O)O1

Mol. weight [g/mol]: 126.15

CAS: 1073-11-6

Physical Properties

Property code	Value	Unit	Source
gf	-81.75	kJ/mol	Joback Method
hf	-256.36	kJ/mol	Joback Method
hfus	7.73	kJ/mol	Joback Method
hvap	38.37	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.268		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
rinpol	1046.00		NIST Webbook
rinpol	996.80		NIST Webbook
rinpol	996.80		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1039.00		NIST Webbook

rinpol	1042.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1035.00		NIST Webbook
ripol	1679.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1689.00		NIST Webbook
ripol	1669.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1683.00		NIST Webbook
ripol	1635.00		NIST Webbook
ripol	1690.00		NIST Webbook
tb	466.53	K	Joback Method
tc	695.24	K	Joback Method
tf	296.48	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.01	J/mol×K	466.53	Joback Method
cpg	231.64	J/mol×K	504.65	Joback Method
cpg	244.35	J/mol×K	542.77	Joback Method
cpg	256.23	J/mol×K	580.88	Joback Method
cpg	267.38	J/mol×K	619.00	Joback Method
cpg	277.91	J/mol×K	657.12	Joback Method
cpg	287.91	J/mol×K	695.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1073116&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

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