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

Other names:	2-Hexen-4-olide
	4-Hydroxy-2-hexenoic acid lactone
	5-Ethyl-2(5H)-furanone
	4-Hydroxyhex-2-enoic acid lactone
	5-Ethyl-(5H)-furan-2-one
	5-Ethyldihydro-2(5H)-furanone
	5-ethylfuran-2(5H)-one
Inchi:	InChI=1S/C6H8O2/c1-2-5-3-4-6(7)8-5/h3-5H,2H2,1H3
InchiKey:	GOUILHYTHSOMQJ-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	CCC1C=CC(=O)O1
Mol. weight [g/mol]:	112.13
CAS:	2407-43-4

Physical Properties

Property code	Value	Unit	Source
gf	-142.56	kJ/mol	Joback Method
hf	-318.61	kJ/mol	Joback Method
hfus	13.94	kJ/mol	Joback Method
hvap	38.26	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.878		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
rinpol	968.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	963.00		NIST Webbook
ripol	1757.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1742.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1700.00		NIST Webbook

ripol	1754.00		NIST Webbook
ripol	1734.00		NIST Webbook
ripol	1716.00		NIST Webbook
tb	445.89	K	Joback Method
tc	665.16	K	Joback Method
tf	263.83	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.45	J/mol×K	445.89	Joback Method
cpg	190.10	J/mol×K	482.44	Joback Method
cpg	201.25	J/mol×K	518.98	Joback Method
cpg	211.91	J/mol×K	555.53	Joback Method
cpg	222.06	J/mol×K	592.07	Joback Method
cpg	231.70	J/mol×K	628.62	Joback Method
cpg	240.82	J/mol×K	665.16	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2407434&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