Dehydroacetic Acid

Other names:	2H-Pyran-2,4(3H)-dione, 3-acetyl-6-methyl-
	Dehydracetic acid
	DHA
	DHS
	3-Acetyl-6-Methyldihydropyrandione-2,4(3H)
	4-Hexenoic acid, 2-acetyl-5-hydroxy-3-oxo-, «delta»-lactone
	Methylacetopyronone
	2-Acetyl-5-hydroxy-3-oxo-4-hexenoic acid, «delta»-lactone
	3-Acetyl-6-methyl-2,4(3H)-pyrandione
	3-Acetyl-6-methyl-2H-pyran-2,4(3H)-dione
	3-Acetyl-6-methylpyrandione-2,4
	3-Acetyl-4-hydroxy-6-methyl-2H-pyran-2-one
	3-Acetyl-6-methyl-2H-pyran-2,4(3H)-dione, enol form
	Kyselina dehydroacetova
	DHAA
	3-Acetyl-6-methyl-pyran-2,4-dione
	3-Acetyl-6-methyl-2H-pyran-2,4(3H)-dione, ion(1-)
	3-Acetyl-6-methyl-2,3-dihydropyran-2,4-dione
	Acetic acid, dehydro-
	Biocide 470F
	NSC 8770
Inchi:	InChI=1S/C8H8O4/c1-4-3-6(10)7(5(2)9)8(11)12-4/h3,7H,1-2H3
InchiKey:	PGRHXDWITVMQBC-UHFFFAOYSA-N
Formula:	C8H8O4
SMILES:	CC(=O)C1C(=O)C=C(C)OC1=O
Mol. weight [g/mol]:	168.15
CAS:	520-45-6

Physical Properties

Property code	Value	Unit	Source
gf	-398.96	kJ/mol	Joback Method
hf	-627.80	kJ/mol	Joback Method
hfus	17.74	kJ/mol	Joback Method
hvap	54.53	kJ/mol	Joback Method
log10ws	-0.60		Crippen Method
logp	0.221		Crippen Method

mcvol	119.000	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
tb	543.20	K	NIST Webbook
tc	867.62	K	Joback Method
tf	382.15 ± 3.00	K	NIST Webbook
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.05	J/mol×K	622.59	Joback Method
cpg	314.52	J/mol×K	663.43	Joback Method
cpg	327.21	J/mol×K	704.27	Joback Method
cpg	339.05	J/mol×K	745.11	Joback Method
cpg	349.99	J/mol×K	785.95	Joback Method
cpg	359.94	J/mol×K	826.78	Joback Method
cpg	368.83	J/mol×K	867.62	Joback Method
hvapt	62.10	kJ/mol	453.00	NIST Webbook

Sources

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=C520456&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt: Enthalpy of vaporization at a given temperature

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume