3-Hydroxy-2,2,4-trimethyl-3-pentenoic acid «beta»-lactone

Other names: Dimethylketene-«beta»-lactone dimer
2,2,4-Trimethyl-3-hydroxy-3-pentenoic acid «beta»-lactone
3-Hydroxy-2,4,4-trimethyl-3-pentenoic acid «beta»-lactone
2-Oxetanone, 3,3-dimethyl-4-(1-methylethylidene)-
Dimethylketene dimer
2-Oxetanone, 4-isopropylidene-3,3-dimethyl-
4-Isopropylidene-3,3-dimethyl-2-oxetanone
3,3-Dimethyl-4-(1-methylethylidene)-2-oxetanone
2,2,4-Trimethylpent-3-en-3-olide
NSC 74312
2,2-dimethyl-3-isopropyliden-«beta»-propiolactone

Inchi: InChI=1S/C8H12O2/c1-5(2)6-8(3,4)7(9)10-6/h1-4H3

InchiKey: OKAAPXFKYOTAEN-UHFFFAOYSA-N

Formula: C8H12O2

SMILES: CC(C)=C1OC(=O)C1(C)C

Mol. weight [g/mol]: 140.18

CAS: 3173-79-3

Physical Properties

Property code	Value	Unit	Source
gf	-112.16	kJ/mol	Joback Method
hf	-330.03	kJ/mol	Joback Method
hfus	12.71	kJ/mol	Joback Method
hvap	41.96	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.863		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
tb	443.20	K	NIST Webbook
tc	718.55	K	Joback Method
tf	309.43	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.54	J/mol×K	494.98	Joback Method
cpg	274.88	J/mol×K	532.24	Joback Method
cpg	287.39	J/mol×K	569.50	Joback Method
cpg	299.16	J/mol×K	606.77	Joback Method
cpg	310.32	J/mol×K	644.03	Joback Method
cpg	320.94	J/mol×K	681.29	Joback Method
cpg	331.15	J/mol×K	718.55	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3173793&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume