2-Cyclopenten-1-one, 2-hydroxy-3,5,5-trimethyl

Other names: 2-hydroxy-3,5,5-trimethyl-2-cyclo-pentenone
2-Hydroxy-3,5,5-trimethyl-2-cyclopenten-1-one
Inchi: InChI=1S/C8H12O2/c1-5-4-8(2,3)7(10)6(5)9/h9H,4H2,1-3H3
InchiKey: JLMOFSIIXFOYRP-UHFFFAOYSA-N
Formula: C8H12O2
SMILES: CC1=C(O)C(=O)C(C)(C)C1
Mol. weight [g/mol]: 140.18
CAS: 53263-56-2

Physical Properties

Property code	Value	Unit	Source
gf	-201.17	kJ/mol	Joback Method
hf	-387.82	kJ/mol	Joback Method
hfus	8.15	kJ/mol	Joback Method
hvap	55.05	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.817		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	1040.00		NIST Webbook
rinpol	1040.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1655.00		NIST Webbook
tb	567.08	K	Joback Method
tc	776.99	K	Joback Method
tf	369.56	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.31	J/mol×K	567.08	Joback Method
cpg	293.74	J/mol×K	602.07	Joback Method

cpg	304.63	J/mol×K	637.05	Joback Method
cpg	315.05	J/mol×K	672.04	Joback Method
cpg	325.08	J/mol×K	707.02	Joback Method
cpg	334.79	J/mol×K	742.01	Joback Method
cpg	344.24	J/mol×K	776.99	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53263562&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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