2-Hydroxy-iso-butyrophenone

Other names:	1-Propanone, 2-hydroxy-2-methyl-1-phenyl-
	1-Phenyl-2-hydroxy-2-methylpropan-1-one
	2-Hydroxy-2-methylpropiophenone
	2-Hydroxy-2-methyl-1-phenyl-1-propanone
	2-Hydroxy-2-methyl-1-phenylpropan-1-one
	Darocure-173 (2-Hydroxy-2-methyl-1-phenyl-propanone)
Inchi:	InChI=1S/C10H12O2/c1-10(2,12)9(11)8-6-4-3-5-7-8/h3-7,12H,1-2H3
InchiKey:	XMLYCEVDHLAQEL-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC(C)(O)C(=O)c1ccccc1
Mol. weight [g/mol]:	164.20
CAS:	7473-98-5

Physical Properties

Property code	Value	Unit	Source
gf	-117.17	kJ/mol	Joback Method
hf	-286.76	kJ/mol	Joback Method
hfus	13.97	kJ/mol	Joback Method
hvap	62.26	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.640		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	1278.00		NIST Webbook
tb	597.70	K	Joback Method
tc	809.57	K	Joback Method
tf	342.05	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.24	J/mol×K	597.70	Joback Method
cpg	343.11	J/mol×K	633.01	Joback Method

cpg	354.13	J/mol×K	668.32	Joback Method
cpg	364.35	J/mol×K	703.63	Joback Method
cpg	373.81	J/mol×K	738.95	Joback Method
cpg	382.59	J/mol×K	774.26	Joback Method
cpg	390.72	J/mol×K	809.57	Joback Method
dvisc	0.0065486	Pa×s	342.05	Joback Method
dvisc	0.0021138	Pa×s	384.66	Joback Method
dvisc	0.0008549	Pa×s	427.27	Joback Method
dvisc	0.0004074	Pa×s	469.88	Joback Method
dvisc	0.0002197	Pa×s	512.48	Joback Method
dvisc	0.0001302	Pa×s	555.09	Joback Method
dvisc	0.0000832	Pa×s	597.70	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7473985&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
dvisc: Dynamic viscosity
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume