1-Propanone, 3-hydroxy-1-phenyl-

Other names:	3-Hydroxy-1-phenylpropan-1-one
	3-Hydroxypropiophenone
Inchi:	InChI=1S/C9H10O2/c10-7-6-9(11)8-4-2-1-3-5-8/h1-5,10H,6-7H2
InchiKey:	PQCFUZMQHVIOSM-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	O=C(CCO)c1ccccc1
Mol. weight [g/mol]:	150.17
CAS:	5650-41-9

Physical Properties

Property code	Value	Unit	Source
gf	-128.43	kJ/mol	Joback Method
hf	-257.37	kJ/mol	Joback Method
hfus	18.79	kJ/mol	Joback Method
hvap	61.33	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.252		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
rinpol	1462.00		NIST Webbook
tb	578.05	K	Joback Method
tc	781.24	K	Joback Method
tf	328.36	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.36	J/mol×K	578.05	Joback Method
cpg	291.87	J/mol×K	611.92	Joback Method
cpg	301.73	J/mol×K	645.78	Joback Method
cpg	310.96	J/mol×K	679.65	Joback Method
cpg	319.60	J/mol×K	713.51	Joback Method
cpg	327.67	J/mol×K	747.38	Joback Method

cpg	335.20	J/mol×K	781.24	Joback Method
dvisc	0.0068844	Pa×s	328.36	Joback Method
dvisc	0.0023345	Pa×s	369.98	Joback Method
dvisc	0.0009851	Pa×s	411.59	Joback Method
dvisc	0.0004871	Pa×s	453.20	Joback Method
dvisc	0.0002711	Pa×s	494.82	Joback Method
dvisc	0.0001653	Pa×s	536.43	Joback Method
dvisc	0.0001082	Pa×s	578.05	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=C5650419&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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