

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

cpg	335.20	J/mol×K	781.24	Joback Method
dvisc	0.0068844	Paxs	328.36	Joback Method
dvisc	0.0023345	Paxs	369.98	Joback Method
dvisc	0.0009851	Paxs	411.59	Joback Method
dvisc	0.0004871	Paxs	453.20	Joback Method
dvisc	0.0002711	Paxs	494.82	Joback Method
dvisc	0.0001653	Paxs	536.43	Joback Method
dvisc	0.0001082	Paxs	578.05	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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