

2'-HYDROXYPROPIOPHENONE

Other names:	o-Hydroxypropiophenone 2'-Hydroxypropiophenone 2-Hydroxyphenyl ethyl ketone 1-Propanone, 1-(2-hydroxyphenyl)- o-Propiophenol Propiophenone, 2'-hydroxy- 2-Propionylphenol Propiophenone, o-hydroxy-
Inchi:	InChI=1S/C9H10O2/c1-2-8(10)7-5-3-4-6-9(7)11/h3-6,11H,2H2,1H3
InchiKey:	KDUWXMIHHIVXER-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	CCC(=O)c1ccccc1O
Mol. weight [g/mol]:	150.18

Physical Properties

Property code	Value	Unit	Source
hf	-312.86	kJ/mol	Cheméo Relay (1.0)
hfus	20.49	kJ/mol	Joback Method
hvap	62.01	kJ/mol	Cheméo Relay (1.0)
ie	8.30	eV	Cheméo Relay (1.0)
log10ws	-2.01		Cheméo Relay (1.0)
logp	1.985		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
tb	512.70	K	Cheméo Relay (1.0)
tc	755.96	K	Cheméo Relay (1.0)
tf	308.30	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.64	J/mol×K	566.49	Joback Method
cpg	339.41	J/mol×K	797.35	Joback Method
cpg	331.37	J/mol×K	758.87	Joback Method

cpg	322.80	J/mol×K	720.40	Joback Method
cpg	313.62	J/mol×K	681.92	Joback Method
cpg	303.76	J/mol×K	643.44	Joback Method
cpg	293.13	J/mol×K	604.97	Joback Method
dvisc	0.0002243	Pa×s	472.88	Joback Method
dvisc	0.0000564	Pa×s	566.49	Joback Method
dvisc	0.0000847	Pa×s	535.29	Joback Method
dvisc	0.0001337	Pa×s	504.08	Joback Method
dvisc	0.0017635	Pa×s	379.26	Joback Method
dvisc	0.0004047	Pa×s	441.67	Joback Method
dvisc	0.0007989	Pa×s	410.47	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	423.20	K	11.00	NIST Webbook
tbrp	388.20	K	2.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C610991&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions

ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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