

2-Propen-1-one, 1-phenyl-

Other names:	Acetophenone, 2-methylene- Acrylophenone Ethylene, benzoyl- Ketone, phenyl vinyl Phenyl vinyl ketone Vinyl phenyl ketone 2-Propenophenone 1-Phenyl-2-propen-1-one 3-Oxo-3-phenylpropene NSC 174109
Inchi:	InChI=1S/C9H8O/c1-2-9(10)8-6-4-3-5-7-8/h2-7H,1H2
InchiKey:	KUIZKZHDMPERHR-UHFFFAOYSA-N
Formula:	C9H8O
SMILES:	<chem>C=CC(=O)c1ccccc1</chem>
Mol. weight [g/mol]:	132.16
CAS:	768-03-6

Physical Properties

Property code	Value	Unit	Source
gf	96.23	kJ/mol	Joback Method
hf	20.29	kJ/mol	Joback Method
hfus	13.43	kJ/mol	Joback Method
hvap	43.98	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.055		Crippen Method
mcvol	111.180	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
rinpol	1138.00		NIST Webbook
rinpol	1147.00		NIST Webbook
tb	482.55	K	Joback Method
tc	705.91	K	Joback Method
tf	265.78	K	Joback Method
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.22	J/molxK	482.55	Joback Method
cpg	228.41	J/molxK	519.78	Joback Method
cpg	239.77	J/molxK	557.00	Joback Method
cpg	250.34	J/molxK	594.23	Joback Method
cpg	260.16	J/molxK	631.46	Joback Method
cpg	269.27	J/molxK	668.69	Joback Method
cpg	277.72	J/molxK	705.91	Joback Method
dvisc	0.0027848	Paxs	265.78	Joback Method
dvisc	0.0015013	Paxs	301.91	Joback Method
dvisc	0.0009236	Paxs	338.04	Joback Method
dvisc	0.0006241	Paxs	374.16	Joback Method
dvisc	0.0004518	Paxs	410.29	Joback Method
dvisc	0.0003447	Paxs	446.42	Joback Method
dvisc	0.0002738	Paxs	482.55	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=C768036&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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