2(5H)-Thiophenone, 5-methyl-

Other names:	5-Methyl-2(5H)-thiophenone
Inchi:	InChI=1S/C5H6OS/c1-4-2-3-5(6)7-4/h2-4H,1H3
InchiKey:	QDQVRZPVOVZFMA-UHFFFAOYSA-N
Formula:	C5H6OS
SMILES:	CC1C=CC(=O)S1
Mol. weight [g/mol]:	114.17
CAS:	7210-64-2

Physical Properties

Property code	Value	Unit	Source
gf	-25.00	kJ/mol	Joback Method
hf	-120.71	kJ/mol	Joback Method
hfus	7.03	kJ/mol	Joback Method
hvap	37.33	kJ/mol	Joback Method
ie	9.16 ± 0.05	eV	NIST Webbook
log10ws	-1.43		Crippen Method
logp	1.204		Crippen Method
mcvol	84.070	ml/mol	McGowan Method
pc	4736.62	kPa	Joback Method
rinpol	826.00		NIST Webbook
tb	443.89	K	Joback Method
tc	683.84	K	Joback Method
tf	309.44	K	Joback Method
vc	0.295	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.55	J/mol×K	443.89	Joback Method
cpg	164.15	J/mol×K	483.88	Joback Method
cpg	174.26	J/mol×K	523.87	Joback Method
cpg	183.86	J/mol×K	563.86	Joback Method
cpg	192.96	J/mol×K	603.86	Joback Method
cpg	201.55	J/mol×K	643.85	Joback Method

cpg	209.62	J/mol×K	683.84	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7210642&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
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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