

4,5-dihydro-5-methyl-3(2H)-thiophenone

Other names:	5-methyltetrahydrothiophen-3-one 4,5-dihydro-5-methylthiophen-3(2H)-one Dihydro-5-methyl-3(2H)-thiophenone
Inchi:	InChI=1S/C5H8OS/c1-4-2-5(6)3-7-4/h4H,2-3H2,1H3
InchiKey:	GYAWKNURSWKRNU-UHFFFAOYSA-N
Formula:	C5H8OS
SMILES:	CC1CC(=O)CS1
Mol. weight [g/mol]:	116.18

Physical Properties

Property code	Value	Unit	Source
gf	-54.96	kJ/mol	Joback Method
hf	-178.49	kJ/mol	Joback Method
hfus	5.81	kJ/mol	Joback Method
hvap	37.04	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	1.081		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	4510.35	kPa	Joback Method
rinpol	982.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	999.00		NIST Webbook
tb	444.73	K	Joback Method
tc	682.05	K	Joback Method
tf	308.68	K	Joback Method
vc	0.309	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.02	J/mol×K	444.73	Joback Method
cpg	180.14	J/mol×K	484.28	Joback Method
cpg	191.71	J/mol×K	523.84	Joback Method
cpg	202.73	J/mol×K	563.39	Joback Method
cpg	213.20	J/mol×K	602.94	Joback Method
cpg	223.10	J/mol×K	642.49	Joback Method
cpg	232.43	J/mol×K	682.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R189441&Units=SI
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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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