5-Methyl-3(2H)-dihydrothiophenone

Other names: 5-methyl-3(2H)-thiophenone
Inchi: InChI=1S/C5H6OS/c1-4-2-5(6)3-7-4/h2H,3H2,1H3
InchiKey: ZFBVNLODJBMXPQ-UHFFFAOYSA-N
Formula: C5H6OS
SMILES: CC1=CC(=O)CS1
Mol. weight [g/mol]: 114.17

Physical Properties

Property code	Value	Unit	Source
gf	-26.92	kJ/mol	Joback Method
hf	-111.84	kJ/mol	Joback Method
hfus	5.57	kJ/mol	Joback Method
hvap	38.30	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.206		Crippen Method
mcvol	84.070	ml/mol	McGowan Method
pc	4856.20	kPa	Joback Method
rinpol	996.00		NIST Webbook
rinpol	1042.00		NIST Webbook
tb	453.54	K	Joback Method
tc	695.30	K	Joback Method
tf	326.20	K	Joback Method
vc	0.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.25	J/mol×K	453.54	Joback Method
cpg	162.01	J/mol×K	493.83	Joback Method
cpg	171.33	J/mol×K	534.13	Joback Method
cpg	180.18	J/mol×K	574.42	Joback Method
cpg	188.58	J/mol×K	614.71	Joback Method
cpg	196.52	J/mol×K	655.01	Joback Method
cpg	203.99	J/mol×K	695.30	Joback Method

Sources

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=R189476&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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