4,5-dihydro-2,(4 or 5)-dimethyl-3(2H)-thiophenone

Inchi: InChI=1S/C6H10OS/c1-4-3-8-5(2)6(4)7/h4-5H,3H2,1-2H3
InchiKey: HOMIEGBJQNRINM-UHFFFAOYSA-N
Formula: C6H10OS
SMILES: CC1CSC(C)C1=O
Mol. weight [g/mol]: 130.21

Physical Properties

Property code	Value	Unit	Source
gf	-54.25	kJ/mol	Joback Method
hf	-219.47	kJ/mol	Joback Method
hfus	9.47	kJ/mol	Joback Method
hvap	38.96	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	1.327		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
rinpol	1045.00		NIST Webbook
rinpol	1045.00		NIST Webbook
tb	462.94	K	Joback Method
tc	696.13	K	Joback Method
tf	315.71	K	Joback Method
vc	0.364	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.01	J/mol×K	462.94	Joback Method
cpg	222.94	J/mol×K	501.81	Joback Method
cpg	236.26	J/mol×K	540.67	Joback Method
cpg	248.97	J/mol×K	579.54	Joback Method
cpg	261.06	J/mol×K	618.40	Joback Method
cpg	272.52	J/mol×K	657.27	Joback Method
cpg	283.33	J/mol×K	696.13	Joback Method

Sources

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=R282738&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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