2-methoxy-2-methyl-4,5-dihydro-3(2H)-thiophenon

Inchi: InChI=1S/C6H10O2S/c1-6(8-2)5(7)3-4-9-6/h3-4H2,1-2H3
InchiKey: FCDCVDDFZHJGKZ-UHFFFAOYSA-N
Formula: C6H10O2S
SMILES: COC1(C)SCCC1=O
Mol. weight [g/mol]: 146.21

Physical Properties

Property code	Value	Unit	Source
gf	-157.03	kJ/mol	Joback Method
hf	-316.11	kJ/mol	Joback Method
hfus	3.29	kJ/mol	Joback Method
hvap	40.53	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	1.055		Crippen Method
mcvol	108.330	ml/mol	McGowan Method
pc	4124.99	kPa	Joback Method
rinpol	1074.00		NIST Webbook
ripol	1645.00		NIST Webbook
tb	490.27	K	Joback Method
tc	731.62	K	Joback Method
tf	366.08	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.88	J/mol×K	490.27	Joback Method
cpg	244.06	J/mol×K	530.49	Joback Method
cpg	256.45	J/mol×K	570.72	Joback Method
cpg	268.12	J/mol×K	610.94	Joback Method
cpg	279.19	J/mol×K	651.17	Joback Method
cpg	289.74	J/mol×K	691.39	Joback Method
cpg	299.87	J/mol×K	731.62	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=R169214&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume