2,5-Dihydro-3,4-dimethylthiophen-2-one

Other names: 2,5-Dihydrothiophen-2-one, 3,4-dimethyl
2(5H)-Thiophenone,3,4-dimethyl-
Inchi: InChI=1S/C6H8OS/c1-4-3-8-6(7)5(4)2/h3H2,1-2H3
InchiKey: IXXRQTNARJNVHF-UHFFFAOYSA-N
Formula: C6H8OS
SMILES: CC1=C(C)C(=O)SC1
Mol. weight [g/mol]: 128.19
CAS: 33922-75-7

Physical Properties

Property code	Value	Unit	Source
gf	-28.13	kJ/mol	Joback Method
hf	-143.95	kJ/mol	Joback Method
hfus	7.77	kJ/mol	Joback Method
hvap	41.19	kJ/mol	Joback Method
ie	9.44 ± 0.05	eV	NIST Webbook
log10ws	-1.74		Crippen Method
logp	1.596		Crippen Method
mcvol	98.160	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
rinpol	1193.00		NIST Webbook
rinpol	1217.00		NIST Webbook
rinpol	1200.00		NIST Webbook
tb	481.40	K	Joback Method
tc	720.36	K	Joback Method
tf	349.99	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.02	J/mol×K	481.40	Joback Method
cpg	201.89	J/mol×K	521.23	Joback Method
cpg	212.30	J/mol×K	561.05	Joback Method

cpg	222.23	J/mol×K	600.88	Joback Method
cpg	231.67	J/mol×K	640.71	Joback Method
cpg	240.62	J/mol×K	680.54	Joback Method
cpg	249.07	J/mol×K	720.36	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=C33922757&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