3.4-dimethyl-2,5-dioxo-2,5-dihydrothiophene

Other names: Thiophene, 2,5-dihydro-2,5-dioxo-3,4-dimethyl
Inchi: InChI=1S/C6H6O2S/c1-3-4(2)6(8)9-5(3)7/h1-2H3
InchiKey: QINKKBMLWVZGGQ-UHFFFAOYSA-N
Formula: C6H6O2S
SMILES: CC1=C(C)C(=O)SC1=O
Mol. weight [g/mol]: 142.18

Physical Properties

Property code	Value	Unit	Source
gf	-150.72	kJ/mol	Joback Method
hf	-281.65	kJ/mol	Joback Method
hfus	7.28	kJ/mol	Joback Method
hvap	45.44	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.123		Crippen Method
mcvol	99.730	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
rinpol	1104.00		NIST Webbook
tb	549.22	K	Joback Method
tc	805.17	K	Joback Method
tf	418.21	K	Joback Method
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.13	J/mol×K	549.22	Joback Method
cpg	218.89	J/mol×K	591.88	Joback Method
cpg	229.25	J/mol×K	634.54	Joback Method
cpg	239.15	J/mol×K	677.19	Joback Method
cpg	248.53	J/mol×K	719.85	Joback Method
cpg	257.33	J/mol×K	762.51	Joback Method
cpg	265.48	J/mol×K	805.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322286&Units=SI
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

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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