3,4-Dimethyldihydrothiophene-2,5-dione

Inchi: InChI=1S/C6H8O2S/c1-3-4(2)6(8)9-5(3)7/h3-4H,1-2H3
InchiKey: MRCQXSVMFJCZIB-UHFFFAOYSA-N
Formula: C6H8O2S
SMILES: CC1C(=O)SC(=O)C1C
Mol. weight [g/mol]: 144.19
CAS: 171917-62-7

Physical Properties

Property code	Value	Unit	Source
gf	-176.84	kJ/mol	Joback Method
hf	-357.17	kJ/mol	Joback Method
hfus	8.98	kJ/mol	Joback Method
hvap	43.20	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	1.059		Crippen Method
mcvol	104.030	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
rinpol	1112.60		NIST Webbook
rinpol	1112.60		NIST Webbook
tb	530.76	K	Joback Method
tc	781.66	K	Joback Method
tf	383.93	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.86	J/mol×K	530.76	Joback Method
cpg	245.59	J/mol×K	572.58	Joback Method
cpg	258.77	J/mol×K	614.39	Joback Method
cpg	271.35	J/mol×K	656.21	Joback Method
cpg	283.25	J/mol×K	698.03	Joback Method
cpg	294.42	J/mol×K	739.84	Joback Method
cpg	304.78	J/mol×K	781.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C171917627&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