1,2-Dithian-4-one, 3,5-dimethyl, #1 (E or Z)

Inchi: InChI=1S/C6H10OS2/c1-4-3-8-9-5(2)6(4)7/h4-5H,3H2,1-2H3
InchiKey: SSIXEKSDRWGGOH-UHFFFAOYSA-N
Formula: C6H10OS2
SMILES: CC1CSSC(C)C1=O
Mol. weight [g/mol]: 162.27

Physical Properties

Property code	Value	Unit	Source
gf	-26.49	kJ/mol	Joback Method
hf	-180.37	kJ/mol	Joback Method
hfus	11.03	kJ/mol	Joback Method
hvap	44.94	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.975		Crippen Method
mcvol	118.810	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
rinpol	1251.00		NIST Webbook
rinpol	1251.00		NIST Webbook
tb	515.04	K	Joback Method
tc	772.76	K	Joback Method
tf	395.64	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.18	J/mol×K	515.04	Joback Method
cpg	266.35	J/mol×K	557.99	Joback Method
cpg	280.73	J/mol×K	600.95	Joback Method
cpg	294.30	J/mol×K	643.90	Joback Method
cpg	307.04	J/mol×K	686.85	Joback Method
cpg	318.93	J/mol×K	729.81	Joback Method
cpg	329.93	J/mol×K	772.76	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=R90313&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