

1,2-Dithian-4-one, 3,5-dimethyl, #2 (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	1261.00		NIST Webbook
rinpol	1261.00		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/molxK	515.04	Joback Method
cpg	266.35	J/molxK	557.99	Joback Method
cpg	280.73	J/molxK	600.95	Joback Method
cpg	294.30	J/molxK	643.90	Joback Method
cpg	307.04	J/molxK	686.85	Joback Method
cpg	318.93	J/molxK	729.81	Joback Method
cpg	329.93	J/molxK	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=R90327&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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