6-methyl-1,2-dithian-4-one

Other names: 3-methyl-5-oxo-1,2-dithiane
Inchi: InChI=1S/C5H8OS2/c1-4-2-5(6)3-7-8-4/h4H,2-3H2,1H3
InchiKey: DDOJKYHUVKAEHQ-UHFFFAOYSA-N
Formula: C5H8OS2
SMILES: CC1CC(=O)CSS1
Mol. weight [g/mol]: 148.25

Physical Properties

Property code	Value	Unit	Source
gf	-27.20	kJ/mol	Joback Method
hf	-139.39	kJ/mol	Joback Method
hfus	7.36	kJ/mol	Joback Method
hvap	43.02	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.729		Crippen Method
mcvol	104.720	ml/mol	McGowan Method
pc	4627.70	kPa	Joback Method
rinpol	1246.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1251.00		NIST Webbook
tb	496.83	K	Joback Method
tc	760.16	K	Joback Method
tf	388.61	K	Joback Method
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.21	J/mol×K	496.83	Joback Method
cpg	220.54	J/mol×K	540.72	Joback Method
cpg	233.18	J/mol×K	584.61	Joback Method
cpg	245.08	J/mol×K	628.49	Joback Method
cpg	256.25	J/mol×K	672.38	Joback Method

cpg	266.65	J/mol×K	716.27	Joback Method
cpg	276.26	J/mol×K	760.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R220047&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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