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

Other names: 1,2-Dithian-4-one, 3-methyl
3-methyl-4-oxo-1,2-dithiane
1,2-Dithian, 3-methyl-4-oxo
Inchi: InChI=1S/C5H8OS2/c1-4-5(6)2-3-7-8-4/h4H,2-3H2,1H3
InchiKey: HIPRPYCXKYSMOO-UHFFFAOYSA-N
Formula: C5H8OS2
SMILES: CC1SSCCC1=O
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	1216.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1241.00		NIST Webbook
ripol	1896.00		NIST Webbook
ripol	1885.00		NIST Webbook
ripol	1864.00		NIST Webbook
ripol	1885.00		NIST Webbook

ripol	1896.00		NIST Webbook
ripol	1864.00		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

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=R640436&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume