4-Methyl-5-oxo-1,2-dithia-3-cyclopentene

Inchi: InChI=1S/C3H4OS2/c1-3-2-5-6-4-3/h2H,1H3
InchiKey: KJBROCNTQJIAAF-UHFFFAOYSA-N
Formula: C3H4OS2
SMILES: CC1=CSSO1
Mol. weight [g/mol]: 120.19

Physical Properties

Property code	Value	Unit	Source
gf	32.57	kJ/mol	Joback Method
hf	-19.60	kJ/mol	Joback Method
hfus	12.52	kJ/mol	Joback Method
hvap	39.93	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.174		Crippen Method
mcvol	76.540	ml/mol	McGowan Method
pc	5981.40	kPa	Joback Method
rinpol	1213.00		NIST Webbook
rinpol	1213.00		NIST Webbook
tb	414.74	K	Joback Method
tc	658.40	K	Joback Method
tf	345.46	K	Joback Method
vc	0.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.97	J/mol×K	414.74	Joback Method
cpg	131.94	J/mol×K	455.35	Joback Method
cpg	138.40	J/mol×K	495.96	Joback Method
cpg	144.37	J/mol×K	536.57	Joback Method
cpg	149.89	J/mol×K	577.18	Joback Method
cpg	155.00	J/mol×K	617.79	Joback Method
cpg	159.72	J/mol×K	658.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R157172&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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