5-Oxo-1,2-dithia-3-cyclopentene

Inchi: InChI=1S/C2H2OS2/c1-2-4-5-3-1/h1-2H
InchiKey: JBPWRHDFVVEDTJ-UHFFFAOYSA-N
Formula: C2H2OS2
SMILES: C1=CSSO1
Mol. weight [g/mol]: 106.17

Physical Properties

Property code	Value	Unit	Source
gf	33.78	kJ/mol	Joback Method
hf	12.51	kJ/mol	Joback Method
hfus	10.31	kJ/mol	Joback Method
hvap	37.04	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.784		Crippen Method
mcvol	62.450	ml/mol	McGowan Method
pc	7157.56	kPa	Joback Method
rinpol	1168.00		NIST Webbook
rinpol	1168.00		NIST Webbook
tb	386.88	K	Joback Method
tc	632.11	K	Joback Method
tf	321.67	K	Joback Method
vc	0.189	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	91.61	J/mol×K	386.88	Joback Method
cpg	97.39	J/mol×K	427.75	Joback Method
cpg	102.64	J/mol×K	468.62	Joback Method
cpg	107.39	J/mol×K	509.49	Joback Method
cpg	111.70	J/mol×K	550.36	Joback Method
cpg	115.58	J/mol×K	591.23	Joback Method
cpg	119.09	J/mol×K	632.11	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=R157494&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume