3-methyl-2-oxothiacyclobutane

Inchi: InChI=1S/C4H6OS/c1-3-2-6-4(3)5/h3H,2H2,1H3
InchiKey: KANHTMXMAWADED-UHFFFAOYSA-N
Formula: C4H6OS
SMILES: CC1CSC1=O
Mol. weight [g/mol]: 102.16

Physical Properties

Property code	Value	Unit	Source
gf	-51.28	kJ/mol	Joback Method
hf	-151.69	kJ/mol	Joback Method
hfus	5.32	kJ/mol	Joback Method
hvap	34.64	kJ/mol	Joback Method
log10ws	-0.81		Crippen Method
logp	0.896		Crippen Method
mcvol	74.280	ml/mol	McGowan Method
pc	4973.33	kPa	Joback Method
rinpol	885.00		NIST Webbook
rinpol	885.00		NIST Webbook
tb	417.58	K	Joback Method
tc	648.58	K	Joback Method
tf	300.93	K	Joback Method
vc	0.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.46	J/mol×K	417.58	Joback Method
cpg	142.00	J/mol×K	456.08	Joback Method
cpg	151.13	J/mol×K	494.58	Joback Method
cpg	159.84	J/mol×K	533.08	Joback Method
cpg	168.14	J/mol×K	571.58	Joback Method
cpg	176.02	J/mol×K	610.08	Joback Method
cpg	183.49	J/mol×K	648.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R156699&Units=SI

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