4,4-Dimethyl thiacyclobutan-2-one

Inchi: InChI=1S/C5H8OS/c1-5(2)3-4(6)7-5/h3H2,1-2H3
InchiKey: BHMHGGHJMPCCSZ-UHFFFAOYSA-N
Formula: C5H8OS
SMILES: CC1(C)CC(=O)S1
Mol. weight [g/mol]: 116.18

Physical Properties

Property code	Value	Unit	Source
gf	-48.35	kJ/mol	Joback Method
hf	-157.09	kJ/mol	Joback Method
hfus	1.61	kJ/mol	Joback Method
hvap	35.72	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.428		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	4634.00	kPa	Joback Method
ripol	1346.00		NIST Webbook
ripol	1346.00		NIST Webbook
tb	440.70	K	Joback Method
tc	679.18	K	Joback Method
tf	336.10	K	Joback Method
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.38	J/mol×K	440.70	Joback Method
cpg	181.69	J/mol×K	480.45	Joback Method
cpg	192.12	J/mol×K	520.19	Joback Method
cpg	201.79	J/mol×K	559.94	Joback Method
cpg	210.80	J/mol×K	599.69	Joback Method
cpg	219.28	J/mol×K	639.43	Joback Method
cpg	227.34	J/mol×K	679.18	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=R239719&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume