2H-Thiopyran, tetrahydro-, 1,1-dioxide

Other names:	Pentamethylene sulfone
	Thiacyclohexane dioxide
	Thiacyclohexane 1,1-dioxide
Inchi:	InChI=1S/C5H10O2S/c6-8(7)4-2-1-3-5-8/h1-5H2
InchiKey:	BUGOPWGPQGYYGR-UHFFFAOYSA-N
Formula:	C5H10O2S
SMILES:	O=S1(=O)CCCCC1
Mol. weight [g/mol]:	134.20
CAS:	4988-33-4

Physical Properties

Property code	Value	Unit	Source
gf	-438.42	kJ/mol	Joback Method
hf	-521.83	kJ/mol	Joback Method
hfus	10.37	kJ/mol	Joback Method
hvap	45.09	kJ/mol	Joback Method
ie	10.24	eV	NIST Webbook
log10ws	-0.64		Crippen Method
logp	0.585		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	5670.27	kPa	Joback Method
tb	364.85	K	Joback Method
tc	556.85	K	Joback Method
tf	371.00 ± 2.00	K	NIST Webbook
tf	374.40 ± 1.00	K	NIST Webbook
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.30	J/mol×K	364.85	Joback Method
cpg	176.71	J/mol×K	396.85	Joback Method
cpg	189.49	J/mol×K	428.85	Joback Method
cpg	201.65	J/mol×K	460.85	Joback Method

cpg	213.20	J/mol×K	492.85	Joback Method
cpg	224.16	J/mol×K	524.85	Joback Method
cpg	234.54	J/mol×K	556.85	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=C4988334&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume