Thiophen-3(2H)-one, dihydro-5-methyl

Other names: «gamma»-Thiovalerolactone
Inchi: InChI=1S/C5H8OS/c1-4-2-3-5(6)7-4/h4H,2-3H2,1H3
InchiKey: BNHNVGAUODLKKT-UHFFFAOYSA-N
Formula: C5H8OS
SMILES: CC1CCC(=O)S1
Mol. weight [g/mol]: 116.18

Physical Properties

Property code	Value	Unit	Source
gf	-54.96	kJ/mol	Joback Method
hf	-178.49	kJ/mol	Joback Method
hfus	5.81	kJ/mol	Joback Method
hvap	37.04	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.428		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	4510.35	kPa	Joback Method
rinpol	982.00		NIST Webbook
rinpol	982.00		NIST Webbook
tb	444.73	K	Joback Method
tc	682.05	K	Joback Method
tf	308.68	K	Joback Method
vc	0.309	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.02	J/mol×K	444.73	Joback Method
cpg	180.14	J/mol×K	484.28	Joback Method
cpg	191.71	J/mol×K	523.84	Joback Method
cpg	202.73	J/mol×K	563.39	Joback Method
cpg	213.20	J/mol×K	602.94	Joback Method
cpg	223.10	J/mol×K	642.49	Joback Method
cpg	232.43	J/mol×K	682.05	Joback Method

Sources

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=U121704&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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