

2,2,3-Trimethyl-thiirane

Other names:	Trimethylthiirane
Inchi:	InChI=1S/C5H10S/c1-4-5(2,3)6-4/h4H,1-3H3
InchiKey:	TWNJQGQIVBDVAB-UHFFFAOYSA-N
Formula:	C5H10S
SMILES:	CC1SC1(C)C
Mol. weight [g/mol]:	102.20
CAS:	53971-47-4

Physical Properties

Property code	Value	Unit	Source
chl	-3938.20	kJ/mol	NIST Webbook
gf	78.63	kJ/mol	Joback Method
hf	-33.57	kJ/mol	Joback Method
hfl	-61.00 ± 1.00	kJ/mol	NIST Webbook
hfus	5.27	kJ/mol	Joback Method
hvap	30.99	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.900		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
rinpol	723.00		NIST Webbook
tb	363.94	K	Joback Method
tc	569.72	K	Joback Method
tf	267.16	K	Joback Method
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.72	J/mol×K	363.94	Joback Method
cpg	162.08	J/mol×K	398.24	Joback Method
cpg	173.37	J/mol×K	432.53	Joback Method
cpg	183.69	J/mol×K	466.83	Joback Method
cpg	193.15	J/mol×K	501.13	Joback Method

cpg	201.85	J/mol×K	535.42	Joback Method
cpg	209.89	J/mol×K	569.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53971474&Units=SI
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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

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