

cis-Dimethylthiirane

Other names: 2,3-Dimethyl-thiirane (Z)
cis-2,3-dimethylthiirane

Inchi: InChI=1S/C4H8S/c1-3-4(2)5-3/h3-4H,1-2H3

InchiKey: ZMJBHClEMIVIFZ-UHFFFAOYSA-N

Formula: C4H8S

SMILES: CC1SC1C

Mol. weight [g/mol]: 88.17

CAS: 5954-71-2

Physical Properties

Property code	Value	Unit	Source
chl	-3295.00 ± 1.00	kJ/mol	NIST Webbook
gf	75.70	kJ/mol	Joback Method
hf	-28.17	kJ/mol	Joback Method
hfl	-24.00 ± 1.00	kJ/mol	NIST Webbook
hfus	8.98	kJ/mol	Joback Method
hvap	29.91	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.510		Crippen Method
mcpol	72.710	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
rinpol	695.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	695.00		NIST Webbook
tb	340.82	K	Joback Method
tc	537.89	K	Joback Method
tf	231.99	K	Joback Method
vc	0.262	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.68	J/mol×K	340.82	Joback Method

cpg	125.45	J/mol×K	373.67	Joback Method
cpg	134.70	J/mol×K	406.51	Joback Method
cpg	143.43	J/mol×K	439.36	Joback Method
cpg	151.68	J/mol×K	472.20	Joback Method
cpg	159.48	J/mol×K	505.05	Joback Method
cpg	166.84	J/mol×K	537.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5954712&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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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