cis-2,3-Dimethylthiophane

Other names: cis-2,3-Dimethyl-thiacyclopentane
2,3-Dimethyltetrahydrothiophene, (Z)-
Inchi: InChI=1S/C6H12S/c1-5-3-4-7-6(5)2/h5-6H,3-4H2,1-2H3/t5-,6-/m0/s1
InchiKey: PQAQKWCWCGKBDS-WDSKDSINSA-N
Formula: C6H12S
SMILES: CC1CCSC1C
Mol. weight [g/mol]: 116.22
CAS: 5161-77-3

Physical Properties

Property code	Value	Unit	Source
gf	68.34	kJ/mol	Joback Method
hf	-81.77	kJ/mol	Joback Method
hfus	9.96	kJ/mol	Joback Method
hvap	34.71	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	2.148		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
rinpol	980.00		NIST Webbook
rinpol	980.00		NIST Webbook
tb	395.12	K	Joback Method
tc	607.56	K	Joback Method
tf	247.49	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.26	J/mol×K	395.12	Joback Method
cpg	196.77	J/mol×K	430.53	Joback Method
cpg	210.55	J/mol×K	465.93	Joback Method
cpg	223.63	J/mol×K	501.34	Joback Method
cpg	236.02	J/mol×K	536.74	Joback Method

cpg	247.76	J/mol×K	572.15	Joback Method
cpg	258.85	J/mol×K	607.56	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=C5161773&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume