Thiophene, tetrahydro-2,5-dimethyl-, trans-

Other names:	trans-2,5-Dimethylthiophane
	2,5-Dimethyl-thiolane (E)
	trans-2,5-Dimethyl-thiacyclopentane
	2,5-Dimethyltetrahydrothiophene, (E)
	trans 2,5-dimethyltetrahydrothiophene
Inchi:	InChI=1S/C6H12S/c1-5-3-4-6(2)7-5/h5-6H,3-4H2,1-2H3/t5-,6-/m0/s1
InchiKey:	IBKCTZVPGMUZGZ-WDSKDSINSA-N
Formula:	C6H12S
SMILES:	CC1CCC(C)S1
Mol. weight [g/mol]:	116.22
CAS:	5161-14-8

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	-2.34		Crippen Method
logp	2.290		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
rinpol	865.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	881.00		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
hvapt	39.30	kJ/mol	372.00	NIST Webbook

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=C5161148&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
hvapt:	Enthalpy of vaporization at a given temperature
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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