

Thiophene, 2,3-dihydro-5-methyl-

Other names:	Thiophene,-2-methyl 4,5-dihydro- 2,3-Dihydro-5-methyl-thiophene 2-Methyl-4,5-dihydrothiophene
Inchi:	InChI=1S/C5H8S/c1-5-3-2-4-6-5/h3H,2,4H2,1H3
InchiKey:	KBUVXRDFMQNIPD-UHFFFAOYSA-N
Formula:	C5H8S
SMILES:	CC1=CCCS1
Mol. weight [g/mol]:	100.18
CAS:	4610-02-0

Physical Properties

Property code	Value	Unit	Source
gf	95.67	kJ/mol	Joback Method
hf	25.86	kJ/mol	Joback Method
hfus	6.06	kJ/mol	Joback Method
hvap	34.06	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.027		Crippen Method
mcvol	82.500	ml/mol	McGowan Method
pc	4627.70	kPa	Joback Method
ripol	847.00		NIST Webbook
ripol	826.00		NIST Webbook
ripol	847.00		NIST Webbook
ripol	823.00		NIST Webbook
ripol	824.00		NIST Webbook
ripol	826.00		NIST Webbook
ripol	824.00		NIST Webbook
ripol	857.00		NIST Webbook
ripol	853.00		NIST Webbook
ripol	823.00		NIST Webbook
ripol	826.00		NIST Webbook
ripol	1142.00		NIST Webbook
ripol	1156.00		NIST Webbook
ripol	1142.00		NIST Webbook
ripol	1148.00		NIST Webbook
ripol	1148.00		NIST Webbook
tb	385.72	K	Joback Method

tc	605.50	K	Joback Method
tf	257.98	K	Joback Method
vc	0.289	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.47	J/mol×K	385.72	Joback Method
cpg	144.02	J/mol×K	422.35	Joback Method
cpg	153.93	J/mol×K	458.98	Joback Method
cpg	163.24	J/mol×K	495.61	Joback Method
cpg	171.96	J/mol×K	532.24	Joback Method
cpg	180.14	J/mol×K	568.87	Joback Method
cpg	187.80	J/mol×K	605.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4610020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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