Thiophene, 2,3-dihydro-

Other names: 2,3-Dihydrothiophene
Dihydro-2-(3H)-thiophene
Inchi: InChI=1S/C4H6S/c1-2-4-5-3-1/h1,3H,2,4H2
InchiKey: OXBLVCZKDOZZOJ-UHFFFAOYSA-N
Formula: C4H6S
SMILES: C1=CSCC1
Mol. weight [g/mol]: 86.16
CAS: 1120-59-8

Physical Properties

Property code	Value	Unit	Source
chl	-3086.80 ± 1.00	kJ/mol	NIST Webbook
gf	96.88	kJ/mol	Joback Method
hf	90.70 ± 1.30	kJ/mol	NIST Webbook
hfl	52.90 ± 1.20	kJ/mol	NIST Webbook
hfus	3.86	kJ/mol	Joback Method
hvap	37.70 ± 0.40	kJ/mol	NIST Webbook
hvap	37.80	kJ/mol	NIST Webbook
hvap	37.79	kJ/mol	NIST Webbook
ie	8.11	eV	NIST Webbook
log10ws	-1.62		Crippen Method
logp	1.637		Crippen Method
mcvol	68.410	ml/mol	McGowan Method
pc	5414.53	kPa	Joback Method
rinpol	780.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	768.00		NIST Webbook
ripol	1104.00		NIST Webbook
tb	385.15 ± 0.60	K	NIST Webbook
tb	385.20	K	NIST Webbook
tc	577.67	K	Joback Method
tf	163.55 ± 1.00	K	NIST Webbook
tf	164.45 ± 1.50	K	NIST Webbook
vc	0.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.73	J/mol×K	541.03	Joback Method
cpg	97.88	J/mol×K	357.86	Joback Method
cpg	107.49	J/mol×K	394.49	Joback Method
cpg	116.44	J/mol×K	431.13	Joback Method
cpg	124.78	J/mol×K	467.76	Joback Method
cpg	132.53	J/mol×K	504.40	Joback Method
cpg	146.41	J/mol×K	577.67	Joback Method
hvapt	33.24	kJ/mol	385.20	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1120598&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
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
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