2-Methyl-4,5-dihydro-3-furanthiol

Other names: Furan-3-thiol, 4,5-dihydro-2-methyl
2-Methyl-4,5(2H)-Furanthiol-3
Inchi: InChI=1S/C5H8OS/c1-4-5(7)2-3-6-4/h7H,2-3H2,1H3
InchiKey: IHRSRTFITLMUQC-UHFFFAOYSA-N
Formula: C5H8OS
SMILES: CC1=C(S)CCO1
Mol. weight [g/mol]: 116.18

Physical Properties

Property code	Value	Unit	Source
gf	-10.55	kJ/mol	Joback Method
hf	-124.39	kJ/mol	Joback Method
hfus	14.03	kJ/mol	Joback Method
hvap	40.15	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.568		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	4931.51	kPa	Joback Method
rinpol	927.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	919.00		NIST Webbook
tb	432.68	K	Joback Method
tc	664.40	K	Joback Method
tf	250.08	K	Joback Method
vc	0.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.59	J/mol×K	432.68	Joback Method
cpg	171.74	J/mol×K	471.30	Joback Method
cpg	181.31	J/mol×K	509.92	Joback Method

cpg	190.31	J/mol×K	548.54	Joback Method
cpg	198.77	J/mol×K	587.16	Joback Method
cpg	206.71	J/mol×K	625.78	Joback Method
cpg	214.15	J/mol×K	664.40	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=R169096&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