3-Furanthiol, dihydro, 2-methyl

Inchi: InChI=1S/C5H8S2/c1-4-5(6)2-3-7-4/h2-6H,1H3
InchiKey: BJWFEVOBXCAJHD-UHFFFAOYSA-N
Formula: C5H8S2
SMILES: CC1SC=CC1S
Mol. weight [g/mol]: 132.25

Physical Properties

Property code	Value	Unit	Source
gf	119.27	kJ/mol	Joback Method
hf	35.13	kJ/mol	Joback Method
hfus	12.63	kJ/mol	Joback Method
hvap	39.51	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.934		Crippen Method
mcvol	98.850	ml/mol	McGowan Method
pc	4710.65	kPa	Joback Method
rinpol	860.00		NIST Webbook
rinpol	860.00		NIST Webbook
tb	434.26	K	Joback Method
tc	680.43	K	Joback Method
tf	273.44	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.37	J/mol×K	434.26	Joback Method
cpg	188.73	J/mol×K	475.29	Joback Method
cpg	200.29	J/mol×K	516.32	Joback Method
cpg	211.08	J/mol×K	557.34	Joback Method
cpg	221.15	J/mol×K	598.37	Joback Method
cpg	230.51	J/mol×K	639.40	Joback Method
cpg	239.20	J/mol×K	680.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R69724&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

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