2,5-Dihydrothiazole

Inchi: InChI=1S/C3H5NS/c1-2-5-3-4-1/h1H,2-3H2
InchiKey: JLPUISACQXFVRC-UHFFFAOYSA-N
Formula: C3H5NS
SMILES: C1=NCSC1
Mol. weight [g/mol]: 87.14

Physical Properties

Property code	Value	Unit	Source
gf	205.24	kJ/mol	Joback Method
hf	149.58	kJ/mol	Joback Method
hfus	6.41	kJ/mol	Joback Method
hvap	35.15	kJ/mol	Joback Method
log10ws	-0.52		Crippen Method
logp	0.761		Crippen Method
mcvol	64.300	ml/mol	McGowan Method
pc	6278.87	kPa	Joback Method
rinpol	826.00		NIST Webbook
rinpol	826.00		NIST Webbook
tb	388.68	K	Joback Method
tc	627.15	K	Joback Method
tf	294.46	K	Joback Method
vc	0.227	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	105.23	J/mol×K	388.68	Joback Method
cpg	115.34	J/mol×K	428.42	Joback Method
cpg	124.83	J/mol×K	468.17	Joback Method
cpg	133.72	J/mol×K	507.91	Joback Method
cpg	142.02	J/mol×K	547.66	Joback Method
cpg	149.75	J/mol×K	587.40	Joback Method
cpg	156.93	J/mol×K	627.15	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=R587216&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