2-methyl-3-thiazoline

Inchi: InChI=1S/C4H7NS/c1-4-5-2-3-6-4/h2,4H,3H2,1H3
InchiKey: GKNTUAWLGAGFEL-UHFFFAOYSA-N
Formula: C4H7NS
SMILES: CC1N=CCS1
Mol. weight [g/mol]: 101.17
CAS: 66867-06-9

Physical Properties

Property code	Value	Unit	Source
gf	205.95	kJ/mol	Joback Method
hf	108.60	kJ/mol	Joback Method
hfus	10.07	kJ/mol	Joback Method
hvap	37.07	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.150		Crippen Method
mcvol	78.390	ml/mol	McGowan Method
pc	5168.28	kPa	Joback Method
ripol	1349.00		NIST Webbook
ripol	1349.00		NIST Webbook
tb	406.89	K	Joback Method
tc	641.82	K	Joback Method
tf	301.49	K	Joback Method
vc	0.281	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	141.92	J/mol×K	406.89	Joback Method
cpg	153.97	J/mol×K	446.04	Joback Method
cpg	165.36	J/mol×K	485.20	Joback Method
cpg	176.10	J/mol×K	524.35	Joback Method
cpg	186.21	J/mol×K	563.51	Joback Method
cpg	195.69	J/mol×K	602.66	Joback Method
cpg	204.55	J/mol×K	641.82	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=C66867069&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume