4-ethyl-2-methyl-3-thiazoline

Inchi: InChI=1S/C6H11NS/c1-3-6-4-8-5(2)7-6/h5H,3-4H2,1-2H3
InchiKey: GBWKVVWPNBCEQA-UHFFFAOYSA-N
Formula: C6H11NS
SMILES: CCC1=NC(C)SC1
Mol. weight [g/mol]: 129.22

Physical Properties

Property code	Value	Unit	Source
gf	213.16	kJ/mol	Joback Method
hf	55.85	kJ/mol	Joback Method
hfus	14.86	kJ/mol	Joback Method
hvap	42.18	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.930		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
rinpol	1061.00		NIST Webbook
rinpol	1061.00		NIST Webbook
tb	457.63	K	Joback Method
tc	687.26	K	Joback Method
tf	336.55	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.77	J/mol×K	457.63	Joback Method
cpg	235.16	J/mol×K	495.90	Joback Method
cpg	248.82	J/mol×K	534.17	Joback Method
cpg	261.73	J/mol×K	572.45	Joback Method
cpg	273.93	J/mol×K	610.72	Joback Method
cpg	285.40	J/mol×K	648.99	Joback Method
cpg	296.17	J/mol×K	687.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R282743&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