2-Acetyl-4,5-dimethyl-2-thiazoline

Inchi: InChI=1S/C7H11NOS/c1-4-6(3)10-7(8-4)5(2)9/h4,6H,1-3H3
InchiKey: XEZCYQPGGHNXSV-UHFFFAOYSA-N
Formula: C7H11NOS
SMILES: CC(=O)C1=NC(C)C(C)S1
Mol. weight [g/mol]: 157.23

Physical Properties

Property code	Value	Unit	Source
gf	84.95	kJ/mol	Joback Method
hf	-97.71	kJ/mol	Joback Method
hfus	20.12	kJ/mol	Joback Method
hvap	50.85	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.498		Crippen Method
mcvol	122.230	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
rinpol	1170.00		NIST Webbook
rinpol	1170.00		NIST Webbook
tb	529.71	K	Joback Method
tc	765.34	K	Joback Method
tf	393.51	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.88	J/mol×K	529.71	Joback Method
cpg	297.75	J/mol×K	568.98	Joback Method
cpg	311.79	J/mol×K	608.25	Joback Method
cpg	324.98	J/mol×K	647.52	Joback Method
cpg	337.35	J/mol×K	686.79	Joback Method
cpg	348.87	J/mol×K	726.07	Joback Method
cpg	359.56	J/mol×K	765.34	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=R329976&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