2H-Thiopyran-3-carboxaldehyde, 5,6-dihydro-2,6-dimethyl-

Other names: 2,6-Dimethyl-5,6-dihydro-2H-thiopyran-3-carbaldehyde
Inchi: InChI=1S/C8H12OS/c1-6-3-4-8(5-9)7(2)10-6/h4-7H,3H2,1-2H3
InchiKey: OVGLVUDQBOCQPR-UHFFFAOYSA-N
Formula: C8H12OS
SMILES: CC1CC=C(C=O)C(C)S1
Mol. weight [g/mol]: 156.25
CAS: 13643-96-4

Physical Properties

Property code	Value	Unit	Source
gf	-6.11	kJ/mol	Joback Method
hf	-168.48	kJ/mol	Joback Method
hfus	16.16	kJ/mol	Joback Method
hvap	47.01	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.026		Crippen Method
mcvol	126.340	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	1240.00		NIST Webbook
rinpol	1240.00		NIST Webbook
tb	497.95	K	Joback Method
tc	722.79	K	Joback Method
tf	321.79	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.04	J/mol×K	497.95	Joback Method
cpg	285.76	J/mol×K	535.42	Joback Method
cpg	299.67	J/mol×K	572.90	Joback Method
cpg	312.80	J/mol×K	610.37	Joback Method
cpg	325.15	J/mol×K	647.84	Joback Method
cpg	336.75	J/mol×K	685.32	Joback Method

cpg	347.61	J/mol×K	722.79	Joback Method

Sources

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=C13643964&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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