2,4-Dimethyl-3,4-dihydro-2H-thiopyran-3-carbalde

Inchi: InChI=1S/C8H12OS/c1-6-3-4-10-7(2)8(6)5-9/h3-8H,1-2H3
InchiKey: WVFWAFOQWGIAOA-UHFFFAOYSA-N
Formula: C8H12OS
SMILES: CC1C=CSC(C)C1C=O
Mol. weight [g/mol]: 156.25

Physical Properties

Property code	Value	Unit	Source
gf	-4.19	kJ/mol	Joback Method
hf	-177.35	kJ/mol	Joback Method
hfus	17.62	kJ/mol	Joback Method
hvap	46.04	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.087		Crippen Method
mcvol	126.340	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
rinpol	1210.00		NIST Webbook
rinpol	1210.00		NIST Webbook
tb	488.30	K	Joback Method
tc	711.68	K	Joback Method
tf	305.03	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.71	J/mol×K	488.30	Joback Method
cpg	287.24	J/mol×K	525.53	Joback Method
cpg	301.92	J/mol×K	562.76	Joback Method
cpg	315.78	J/mol×K	599.99	Joback Method
cpg	328.82	J/mol×K	637.22	Joback Method
cpg	341.05	J/mol×K	674.45	Joback Method
cpg	352.51	J/mol×K	711.68	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=R487280&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