4-Hydroxy-2,6-dimethyl-tetrahydro-thiopyran-3-ca

Inchi: InChI=1S/C8H14O2S/c1-5-3-8(10)7(4-9)6(2)11-5/h4-8,10H,3H2,1-2H3
InchiKey: SBABNVSRZXHIGQ-UHFFFAOYSA-N
Formula: C8H14O2S
SMILES: CC1CC(O)C(C=O)C(C)S1
Mol. weight [g/mol]: 174.26

Physical Properties

Property code	Value	Unit	Source
gf	-178.68	kJ/mol	Joback Method
hf	-407.70	kJ/mol	Joback Method
hfus	21.56	kJ/mol	Joback Method
hvap	62.11	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	1.076		Crippen Method
mcvol	136.510	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	1324.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1342.00		NIST Webbook
tb	576.65	K	Joback Method
tc	781.89	K	Joback Method
tf	360.85	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.01	J/mol×K	576.65	Joback Method
cpg	361.34	J/mol×K	610.86	Joback Method
cpg	374.92	J/mol×K	645.06	Joback Method
cpg	387.75	J/mol×K	679.27	Joback Method
cpg	399.84	J/mol×K	713.48	Joback Method
cpg	411.20	J/mol×K	747.68	Joback Method
cpg	421.83	J/mol×K	781.89	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=R487255&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