trans-Wiskey lactone, thio

Inchi: InChI=1S/C9H16OS/c1-3-4-5-8-7(2)6-9(10)11-8/h7-8H,3-6H2,1-2H3/t7-,8+/m1/s1
InchiKey: MXJQBWKNBCIJHS-SFYZADRCSA-N
Formula: C9H16OS
SMILES: CCCCC1SC(=O)CC1C
Mol. weight [g/mol]: 172.29

Physical Properties

Property code	Value	Unit	Source
gf	-28.99	kJ/mol	Joback Method
hf	-281.39	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	45.64	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.845		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1362.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1926.00		NIST Webbook
tb	531.58	K	Joback Method
tc	752.96	K	Joback Method
tf	349.52	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.22	J/mol×K	531.58	Joback Method
cpg	358.53	J/mol×K	568.48	Joback Method
cpg	375.00	J/mol×K	605.37	Joback Method
cpg	390.63	J/mol×K	642.27	Joback Method
cpg	405.43	J/mol×K	679.17	Joback Method
cpg	419.40	J/mol×K	716.07	Joback Method
cpg	432.53	J/mol×K	752.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R586020&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume