cis-Wiskey lactone, dithio

Inchi: InChI=1S/C9H16S2/c1-3-4-5-8-7(2)6-9(10)11-8/h7-8H,3-6H2,1-2H3/t7-,8-/m0/s1
InchiKey: KRJXCMCPWNDYTN-YUMQZZPRSA-N
Formula: C9H16S2
SMILES: CCCCC1SC(=S)CC1C
Mol. weight [g/mol]: 188.35

Physical Properties

Property code	Value	Unit	Source
gf	184.45	kJ/mol	Joback Method
hf	-28.59	kJ/mol	Joback Method
hfus	23.76	kJ/mol	Joback Method
hvap	48.87	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.646		Crippen Method
mcvol	155.210	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpol	1567.00		NIST Webbook
ripol	2200.00		NIST Webbook
tb	536.40	K	Joback Method
tc	761.38	K	Joback Method
tf	344.97	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.34	J/mol×K	536.40	Joback Method
cpg	365.37	J/mol×K	573.90	Joback Method
cpg	380.42	J/mol×K	611.39	Joback Method
cpg	394.53	J/mol×K	648.89	Joback Method
cpg	407.77	J/mol×K	686.38	Joback Method
cpg	420.19	J/mol×K	723.88	Joback Method
cpg	431.85	J/mol×K	761.38	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=R585978&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume