1,3-Dithiolane, 3-acetyl

Inchi: InChI=1S/C5H8OS2/c1-4(6)5-7-2-3-8-5/h5H,2-3H2,1H3
InchiKey: VDPJAYJVAJMICF-UHFFFAOYSA-N
Formula: C5H8OS2
SMILES: CC(=O)C1SCCS1
Mol. weight [g/mol]: 148.25

Physical Properties

Property code	Value	Unit	Source
gf	-21.43	kJ/mol	Joback Method
hf	-108.11	kJ/mol	Joback Method
hfus	11.55	kJ/mol	Joback Method
hvap	45.35	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.381		Crippen Method
mcvol	104.720	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
tb	478.61	K	Joback Method
tc	723.79	K	Joback Method
tf	373.84	K	Joback Method
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.70	J/mol×K	478.61	Joback Method
cpg	213.54	J/mol×K	519.47	Joback Method
cpg	224.57	J/mol×K	560.34	Joback Method
cpg	234.82	J/mol×K	601.20	Joback Method
cpg	244.34	J/mol×K	642.06	Joback Method
cpg	253.15	J/mol×K	682.93	Joback Method
cpg	261.32	J/mol×K	723.79	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=R78933&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume