3-acetyl-1,2-dithiolane

Other names: 1,2-Dithiolane, 3-acetyl
Inchi: InChI=1S/C5H8OS2/c1-4(6)5-2-3-7-8-5/h5H,2-3H2,1H3
InchiKey: OEBJHVCWENCTLE-UHFFFAOYSA-N
Formula: C5H8OS2
SMILES: CC(=O)C1CCSS1
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	-1.96		Crippen Method
logp	1.729		Crippen Method
mcvol	104.720	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
rinpol	1199.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1208.00		NIST Webbook
ripol	1994.00		NIST Webbook
ripol	1994.00		NIST Webbook
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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R125789&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

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