2-acetylthietane

Inchi: InChI=1S/C5H8OS/c1-4(6)5-2-3-7-5/h5H,2-3H2,1H3
InchiKey: LHLNSXFHEGETML-UHFFFAOYSA-N
Formula: C5H8OS
SMILES: CC(=O)C1CCS1
Mol. weight [g/mol]: 116.18

Physical Properties

Property code	Value	Unit	Source
gf	-49.19	kJ/mol	Joback Method
hf	-147.21	kJ/mol	Joback Method
hfus	10.00	kJ/mol	Joback Method
hvap	39.37	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	1.081		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
rinpol	972.00		NIST Webbook
ripol	1549.00		NIST Webbook
ripol	1549.00		NIST Webbook
tb	426.51	K	Joback Method
tc	646.47	K	Joback Method
tf	293.91	K	Joback Method
vc	0.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.20	J/mol×K	426.51	Joback Method
cpg	174.23	J/mol×K	463.17	Joback Method
cpg	184.56	J/mol×K	499.83	Joback Method
cpg	194.23	J/mol×K	536.49	Joback Method
cpg	203.28	J/mol×K	573.15	Joback Method
cpg	211.74	J/mol×K	609.81	Joback Method
cpg	219.63	J/mol×K	646.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R169190&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