1,3-Oxathiane, 2,5-dimethyl

Inchi: InChI=1S/C6H12OS/c1-5-3-7-6(2)8-4-5/h5-6H,3-4H2,1-2H3
InchiKey: ZDXSSYRUPOPWQI-UHFFFAOYSA-N
Formula: C6H12OS
SMILES: CC1COC(C)SC1
Mol. weight [g/mol]: 132.22

Physical Properties

Property code	Value	Unit	Source
gf	-29.88	kJ/mol	Joback Method
hf	-219.93	kJ/mol	Joback Method
hfus	15.84	kJ/mol	Joback Method
hvap	39.39	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	1.732		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
rinpol	1054.00		NIST Webbook
tb	426.34	K	Joback Method
tc	647.69	K	Joback Method
tf	270.54	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.89	J/mol×K	426.34	Joback Method
cpg	224.99	J/mol×K	463.23	Joback Method
cpg	239.34	J/mol×K	500.12	Joback Method
cpg	252.96	J/mol×K	537.02	Joback Method
cpg	265.86	J/mol×K	573.91	Joback Method
cpg	278.04	J/mol×K	610.80	Joback Method
cpg	289.53	J/mol×K	647.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R63106&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume