1,4-Oxathiane

Other names:	1,4-Oxathiin, 2,3,5,6-tetrahydro-
	1,4-Thioxane
	1-Oxa-4-thiacyclohexane
	1-Thia-4-oxacyclohexane
	NSC 49179
	Oxathiane
	p-Thioxane
Inchi:	InChI=1S/C4H8OS/c1-3-6-4-2-5-1/h1-4H2
InchiKey:	JBYHSSAVUBIJMK-UHFFFAOYSA-N
Formula:	C4H8OS
SMILES:	C1CSCCO1
Mol. weight [g/mol]:	104.17
CAS:	15980-15-1

Physical Properties

Property code	Value	Unit	Source
gf	-31.30	kJ/mol	Joback Method
hf	-137.97	kJ/mol	Joback Method
hfus	8.52	kJ/mol	Joback Method
hvap	35.56	kJ/mol	Joback Method
ie	8.67	eV	NIST Webbook
ie	8.80 ± 0.05	eV	NIST Webbook
log10ws	-0.36		Crippen Method
logp	0.750		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	5258.62	kPa	Joback Method
rinpol	851.00		NIST Webbook
rinpol	884.50		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	897.00		NIST Webbook
tb	389.92	K	Joback Method
tc	617.73	K	Joback Method
tf	251.50 ± 0.60	K	NIST Webbook

vc	0.261	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.36	J/mol×K	389.92	Joback Method
cpg	144.03	J/mol×K	427.89	Joback Method
cpg	155.00	J/mol×K	465.86	Joback Method
cpg	165.30	J/mol×K	503.82	Joback Method
cpg	174.96	J/mol×K	541.79	Joback Method
cpg	184.01	J/mol×K	579.76	Joback Method
cpg	192.46	J/mol×K	617.73	Joback Method
hvapt	42.10	kJ/mol	376.50	NIST Webbook
hvapt	44.80	kJ/mol	376.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	420.20	K	101.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.25550e+01
Coeff. B	-2.40177e+03
Coeff. C	-1.17583e+02
Temperature range (K), min.	313.37
Temperature range (K), max.	449.16

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C15980151&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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume