

1,3-Oxathiolane, 5-methyl-2-(1-methylethyl)-, cis-

Inchi:	InChI=1S/C7H14OS/c1-5(2)7-8-6(3)4-9-7/h5-7H,4H2,1-3H3/t6-,7-/m0/s1
InchiKey:	ODRUEFNMTNWJNO-BQBZGAKWSA-N
Formula:	C7H14OS
SMILES:	CC1CSC(C(C)C)O1
Mol. weight [g/mol]:	146.25
CAS:	38384-68-8

Physical Properties

Property code	Value	Unit	Source
gf	-11.80	kJ/mol	Joback Method
hf	-239.69	kJ/mol	Joback Method
hfus	17.00	kJ/mol	Joback Method
hvap	41.06	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	2.120		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	444.51	K	Joback Method
tc	659.36	K	Joback Method
tf	270.33	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.16	J/molxK	444.51	Joback Method
cpg	267.93	J/molxK	480.32	Joback Method
cpg	282.89	J/molxK	516.13	Joback Method
cpg	297.06	J/molxK	551.94	Joback Method
cpg	310.46	J/molxK	587.75	Joback Method
cpg	323.11	J/molxK	623.56	Joback Method
cpg	335.04	J/molxK	659.36	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C38384688&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/13-626-2/1-3-Oxathiolane-5-methyl-2-1-methylethyl-cis.pdf>

Generated by Cheméo on 2024-04-28 23:17:38.127615383 +0000 UTC m=+16635507.048192695.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.