

1,3-Oxathiane,2,2,4,6-tetramethyl,trans-

Inchi:	InChI=1S/C8H16OS/c1-6-5-7(2)10-8(3,4)9-6/h6-7H,5H2,1-4H3/t6-,7-/m0/s1
InchiKey:	LPCWYDWZCPIOJH-BQBZGAKWSA-N
Formula:	C8H16OS
SMILES:	CC1CC(C)SC(C)(C)O1
Mol. weight [g/mol]:	160.28
CAS:	34560-78-6

Physical Properties

Property code	Value	Unit	Source
gf	-26.24	kJ/mol	Joback Method
hf	-266.31	kJ/mol	Joback Method
hfus	15.79	kJ/mol	Joback Method
hvap	42.38	kJ/mol	Joback Method
ie	8.45 ± 0.01	eV	NIST Webbook
log10ws	-2.87		Crippen Method
logp	2.653		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	467.67	K	Joback Method
tc	692.25	K	Joback Method
tf	312.74	K	Joback Method
vc	0.479	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.75	J/mol×K	467.67	Joback Method
cpg	313.73	J/mol×K	505.10	Joback Method
cpg	330.56	J/mol×K	542.53	Joback Method
cpg	346.34	J/mol×K	579.96	Joback Method
cpg	361.18	J/mol×K	617.39	Joback Method
cpg	375.19	J/mol×K	654.82	Joback Method
cpg	388.47	J/mol×K	692.25	Joback Method

Sources

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=C34560786&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	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.cheméo.com/cid/58-269-0/1-3-Oxathiane-2-2-4-6-tetramethyl-trans.pdf>

Generated by Cheméo on 2024-04-29 22:31:26.38427413 +0000 UTC m=+16719135.304851447.

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