

1,2-OXATHIOLANE, 2,2-DIOXIDE

Other names:	«gamma»-Propane sultone Propane sultone 1-Propanesulfonic acid, 3-hydroxy-, «gamma»-sultone 1,3-Propane sultone 3-Hydroxy-1-propanesulfonic acid, sultone 3-Hydroxy-1-propanesulfonic acid «gamma»-sultone 3-Hydroxy-1-propanesulphonic acid sultone Rcra waste number U193 NSC 42386
Inchi:	InChI=1S/C3H6O3S/c4-7(5)3-1-2-6-7/h1-3H2
InchiKey:	FSSPGSAQUIYDCN-UHFFFAOYSA-N
Formula:	C3H6O3S
SMILES:	O=S1(=O)CCCO1
Mol. weight [g/mol]:	122.14

Physical Properties

Property code	Value	Unit	Source
hfus	15.27	kJ/mol	Joback Method
logp	-0.263		Crippen Method
mcvol	76.230	ml/mol	McGowan Method
tf	304.33 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.62	J/mol×K	341.77	Joback Method
cpg	133.07	J/mol×K	372.86	Joback Method
cpg	142.05	J/mol×K	403.95	Joback Method
cpg	150.59	J/mol×K	435.05	Joback Method
cpg	158.68	J/mol×K	466.14	Joback Method
cpg	166.35	J/mol×K	497.23	Joback Method
cpg	173.60	J/mol×K	528.32	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1120714&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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<https://www.chemeo.com/cid/81-294-6/1-2-OXATHIOLANE-2-2-DIOXIDE.pdf>

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