

1,3,2-Dioxathiolane, 2-oxide

Other names:	1,2-Ethylene sulfite
	1,2-ethanediol, cyclic sulfite
	Cyclic ethylene sulfite
	Ethylene glycol, cyclic sulfite
	Glycol sulfite
	NSC 3225
	Sulfurous acid, cyclic ester with ethylene glycol
	ethylene glycol cyclic sulfite
	ethylene sulfite
	ethylene sulphite
Inchi:	InChI=1S/C2H4O3S/c3-6-4-1-2-5-6/h1-2H2
InchiKey:	WDXYVJKNSMILOQ-UHFFFAOYSA-N
Formula:	C2H4O3S
SMILES:	O=S1OCCO1
Mol. weight [g/mol]:	108.12
CAS:	3741-38-6

Physical Properties

Property code	Value	Unit	Source
ea	0.01 ± 0.00	eV	NIST Webbook
gf	-372.99	kJ/mol	Joback Method
hf	-470.14	kJ/mol	Joback Method
hfus	17.04	kJ/mol	Joback Method
hvap	41.35	kJ/mol	Joback Method
ie	10.30 ± 0.05	eV	NIST Webbook
ie	10.30	eV	NIST Webbook
ie	10.93	eV	NIST Webbook
ie	10.93	eV	NIST Webbook
log10ws	0.65		Crippen Method
logp	-0.388		Crippen Method
mcvol	62.140	ml/mol	McGowan Method
pc	7535.20	kPa	Joback Method
tb	356.34	K	Joback Method
tc	561.40	K	Joback Method
tf	266.11	K	Joback Method
vc	0.213	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	104.54	J/mol×K	356.34	Joback Method
cpg	112.02	J/mol×K	390.52	Joback Method
cpg	119.08	J/mol×K	424.69	Joback Method
cpg	125.71	J/mol×K	458.87	Joback Method
cpg	131.95	J/mol×K	493.05	Joback Method
cpg	137.80	J/mol×K	527.22	Joback Method
cpg	143.27	J/mol×K	561.40	Joback Method
rhoI	1432.17	kg/m3	298.15	Solid-liquid equilibria and thermo-physical properties of liquid electrolyte systems for lithium ion batteries

Sources

Crippen Method:

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

Solid-liquid equilibria and thermo-physical properties of liquid electrolyte systems for lithium ion batteries:

<https://www.doi.org/10.1016/j.fluid.2018.05.033>

Joback Method:
McGowan Method:

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

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3741386&Units=SI>

Crippen Method:

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

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
rho:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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