

2-Ethyl-1,3-oxothiolane

Other names:	2-Ethyl-1,3-thioxalane
Inchi:	InChI=1S/C5H10OS/c1-2-5-6-3-4-7-5/h5H,2-4H2,1H3
InchiKey:	HUNYQOGBLJVUSK-UHFFFAOYSA-N
Formula:	C5H10OS
SMILES:	CCC1OCCS1
Mol. weight [g/mol]:	118.20

Physical Properties

Property code	Value	Unit	Source
gf	-18.49	kJ/mol	Joback Method
hf	-172.79	kJ/mol	Joback Method
hfus	14.28	kJ/mol	Joback Method
hvap	37.30	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.486		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
rinpol	963.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	922.00		NIST Webbook
tb	403.86	K	Joback Method
tc	619.14	K	Joback Method
tf	267.03	K	Joback Method
vc	0.324	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.92	J/mol×K	403.86	Joback Method

cpg	184.40	J/mol×K	439.74	Joback Method
cpg	196.21	J/mol×K	475.62	Joback Method
cpg	207.36	J/mol×K	511.50	Joback Method
cpg	217.87	J/mol×K	547.38	Joback Method
cpg	227.78	J/mol×K	583.26	Joback Method
cpg	237.10	J/mol×K	619.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R78826&Units=SI
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

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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