

1,3-Oxathiolan-2-one

Inchi:	InChI=1S/C3H4O2S/c4-3-5-1-2-6-3/h1-2H2
InchiKey:	DAJDXKBYZZGECL-UHFFFAOYSA-N
Formula:	C3H4O2S
SMILES:	O=C1OCCS1
Mol. weight [g/mol]:	104.13
CAS:	3326-89-4

Physical Properties

Property code	Value	Unit	Source
gf	-150.21	kJ/mol	Joback Method
hf	-248.87	kJ/mol	Joback Method
hfus	7.54	kJ/mol	Joback Method
hvap	37.41	kJ/mol	Joback Method
log10ws	-0.70		Crippen Method
logp	0.870		Crippen Method
mcvol	66.060	ml/mol	McGowan Method
pc	6170.82	kPa	Joback Method
tb	430.59	K	Joback Method
tc	674.50	K	Joback Method
tf	316.95	K	Joback Method
vc	0.220	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.19	J/mol×K	430.59	Joback Method
cpg	125.42	J/mol×K	471.24	Joback Method
cpg	133.29	J/mol×K	511.89	Joback Method
cpg	140.78	J/mol×K	552.54	Joback Method
cpg	147.88	J/mol×K	593.20	Joback Method
cpg	154.58	J/mol×K	633.85	Joback Method
cpg	160.88	J/mol×K	674.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3326894&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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