2-Methyl-1,3-oxathiolane

Other names: 1,3-Oxathiolane, 2-methyl-
2-Methyl-1,3-oxothiolane
Inchi: InChI=1S/C4H8OS/c1-4-5-2-3-6-4/h4H,2-3H2,1H3
InchiKey: QNNPPEKCYFEVCF-UHFFFAOYSA-N
Formula: C4H8OS
SMILES: CC1OCCS1
Mol. weight [g/mol]: 104.17
CAS: 17642-74-9

Physical Properties

Property code	Value	Unit	Source
gf	-26.91	kJ/mol	Joback Method
hf	-152.15	kJ/mol	Joback Method
hfus	11.69	kJ/mol	Joback Method
hvap	35.08	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	1.096		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4842.69	kPa	Joback Method
rinpol	830.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	807.00		NIST Webbook
rinpol	834.00		NIST Webbook
tb	380.98	K	Joback Method
tc	598.45	K	Joback Method
tf	255.76	K	Joback Method
vc	0.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.54	J/mol×K	380.98	Joback Method
cpg	146.53	J/mol×K	417.23	Joback Method
cpg	156.91	J/mol×K	453.47	Joback Method
cpg	166.70	J/mol×K	489.72	Joback Method
cpg	175.93	J/mol×K	525.96	Joback Method
cpg	184.62	J/mol×K	562.21	Joback Method
cpg	192.79	J/mol×K	598.45	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17642749&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
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

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