Thiirane, ethyl-

Other names: 2-Ethyl-thiirane
Inchi: InChI=1S/C4H8S/c1-2-4-3-5-4/h4H,2-3H2,1H3
InchiKey: ZXKFFOMHVCMTEV-UHFFFAOYSA-N
Formula: C4H8S
SMILES: CCC1CS1
Mol. weight [g/mol]: 88.17
CAS: 3195-86-6

Physical Properties

Property code	Value	Unit	Source
gf	83.41	kJ/mol	Joback Method
hf	-7.83	kJ/mol	Joback Method
hfus	7.91	kJ/mol	Joback Method
hvap	30.22	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.512		Crippen Method
mcvol	72.710	ml/mol	McGowan Method
pc	4577.74	kPa	Joback Method
rinpol	727.00		NIST Webbook
rinpol	727.00		NIST Webbook
rinpol	727.00		NIST Webbook
tb	345.49	K	Joback Method
tc	543.36	K	Joback Method
tf	236.23	K	Joback Method
vc	0.263	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.59	J/mol×K	510.38	Joback Method
cpg	114.86	J/mol×K	345.49	Joback Method
cpg	124.51	J/mol×K	378.47	Joback Method
cpg	133.58	J/mol×K	411.45	Joback Method
cpg	142.10	J/mol×K	444.42	Joback Method

cpg	150.09	J/mol×K	477.40	Joback Method
cpg	164.64	J/mol×K	543.36	Joback Method
hvapt	39.70	kJ/mol	374.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3195866&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
hvapt:	Enthalpy of vaporization at a given temperature
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