3-Ethylthiolane

Other names:	3-Ethyltetrahydrothiophene
	3-Ethyl-thiacyclopentane
Inchi:	InChI=1S/C6H12S/c1-2-6-3-4-7-5-6/h6H,2-5H2,1H3
InchiKey:	BEEJXKSVPBKHQM-UHFFFAOYSA-N
Formula:	C6H12S
SMILES:	CCC1CCSC1
Mol. weight [g/mol]:	116.22
CAS:	62184-67-2

Physical Properties

Property code	Value	Unit	Source
gf	76.05	kJ/mol	Joback Method
hf	-61.43	kJ/mol	Joback Method
hfus	8.89	kJ/mol	Joback Method
hvap	35.02	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	2.150		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
rinpol	970.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	970.00		NIST Webbook
tb	399.79	K	Joback Method
tc	612.75	K	Joback Method
tf	251.73	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.81	J/mol×K	399.79	Joback Method
cpg	196.08	J/mol×K	435.28	Joback Method

cpg	209.57	J/mol×K	470.78	Joback Method
cpg	222.32	J/mol×K	506.27	Joback Method
cpg	234.36	J/mol×K	541.76	Joback Method
cpg	245.71	J/mol×K	577.25	Joback Method
cpg	256.40	J/mol×K	612.75	Joback Method
hvapt	43.10	kJ/mol	423.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62184672&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

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