

Thiocyanic acid, ethyl ester

Other names:	Aethylrhodanid Ethane, thiocyanato- Ethyl rhodanate Ethyl sulfocyanate Ethyl thiocyanate Ethylthiokyanat
Inchi:	InChI=1S/C3H5NS/c1-2-5-3-4/h2H2,1H3
InchiKey:	WFCLYEAZTHWNEH-UHFFFAOYSA-N
Formula:	C3H5NS
SMILES:	CCSC#N
Mol. weight [g/mol]:	87.14
CAS:	542-90-5

Physical Properties

Property code	Value	Unit	Source
gf	140.68	kJ/mol	Joback Method
hf	101.50	kJ/mol	Joback Method
hfus	9.16	kJ/mol	Joback Method
hvap	39.57	kJ/mol	Joback Method
ie	9.89 ± 0.01	eV	NIST Webbook
ie	9.77 ± 0.05	eV	NIST Webbook
log10ws	-1.32		Crippen Method
logp	1.221		Crippen Method
mcvol	70.860	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	419.20	K	NIST Webbook
tb	417.55 ± 0.60	K	NIST Webbook
tc	658.75	K	Joback Method
tf	187.65 ± 0.50	K	NIST Webbook
vc	0.283	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	143.73	J/mol×K	622.11	Joback Method
cpg	118.51	J/mol×K	438.90	Joback Method
cpg	124.00	J/mol×K	475.54	Joback Method
cpg	129.27	J/mol×K	512.18	Joback Method
cpg	134.31	J/mol×K	548.82	Joback Method
cpg	139.14	J/mol×K	585.47	Joback Method
cpg	148.09	J/mol×K	658.75	Joback Method
hvapt	44.20	kJ/mol	390.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38871e+01
Coeff. B	-3.09362e+03
Coeff. C	-8.53820e+01
Temperature range (K), min.	312.86
Temperature range (K), max.	446.13

Sources

The Yaws Handbook of Vapor Pressure: Crippen Method:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C542905&Units=SI

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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