

Thiourea, ethyl-

Other names:	1-Ethyl-2-Thiourea 1-Ethylthiourea ENT 61326 N-Ethylthiocarbamide N-Ethylthiourea Urea, 1-ethyl-2-thio-ethyl-2-thiourea ethylthiourea
Inchi:	InChI=1S/C3H8N2S/c1-2-5-3(4)6/h2H2,1H3,(H3,4,5,6)
InchiKey:	GMEHFXXZSWDEDB-UHFFFAOYSA-N
Formula:	C3H8N2S
SMILES:	CCNC(=N)S
Mol. weight [g/mol]:	104.17
CAS:	625-53-6

Physical Properties

Property code	Value	Unit	Source
gf	296.76	kJ/mol	Joback Method
hf	185.03	kJ/mol	Joback Method
hvap	47.53	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	0.460		Crippen Method
mvol	85.140	ml/mol	McGowan Method
tb	465.41	K	Joback Method
tf	281.47	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	39.26	J/molxK	100.12	Joback Method
cpg	39.26	J/molxK	100.12	Joback Method
cpg	39.26	J/molxK	100.12	Joback Method
cpg	39.26	J/molxK	100.12	Joback Method
cpg	39.26	J/molxK	100.12	Joback Method

cpg	161.92	J/mol×K	465.41	Joback Method
cpg	39.26	J/mol×K	100.12	Joback Method
psub	2.82e-04	kPa	356.50	Thermal stability and related thermodynamic properties of N-ethylthiourea
psub	3.09e-04	kPa	357.00	Thermal stability and related thermodynamic properties of N-ethylthiourea
psub	4.17e-04	kPa	360.50	Thermal stability and related thermodynamic properties of N-ethylthiourea
psub	4.90e-04	kPa	362.00	Thermal stability and related thermodynamic properties of N-ethylthiourea
psub	9.12e-04	kPa	367.50	Thermal stability and related thermodynamic properties of N-ethylthiourea

Sources

Thermal stability and related thermodynamic properties of N-ethylthiourea

<https://www.doi.org/10.1016/j.tca.2007.05.009>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C625536&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume
psub: Sublimation pressure
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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