ethylthiourea

Other names: thiourea, ethyl-
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]: 104.18

Physical Properties

Property code	Value	Unit	Source
gf	247.28	kJ/mol	Joback Method
hf	128.51	kJ/mol	Joback Method
hfus	18.43	kJ/mol	Joback Method
hvap	46.08	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	-0.160		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
pc	5536.07	kPa	Joback Method
tb	460.78	K	Joback Method
tc	679.27	K	Joback Method
tf	293.76	K	Joback Method
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.96	J/mol×K	460.78	Joback Method
cpg	172.79	J/mol×K	497.19	Joback Method
cpg	180.05	J/mol×K	533.61	Joback Method
cpg	186.79	J/mol×K	570.02	Joback Method
cpg	193.04	J/mol×K	606.44	Joback Method
cpg	198.86	J/mol×K	642.85	Joback Method
cpg	204.28	J/mol×K	679.27	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	
psub	3.31e-04	kPa	360.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	4.37e-04	kPa	361.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	4.47e-04	kPa	363.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	5.50e-04	kPa	364.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	6.61e-04	kPa	365.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	6.31e-04	kPa	366.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	8.13e-04	kPa	366.50	Thermal stability and related thermodynamic properties of N-ethylthiourea	

psub	7.41e-04	kPa	367.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	9.12e-04	kPa	368.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	6.46e-04	kPa	368.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	7.94e-04	kPa	368.50	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	8.91e-04	kPa	369.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.18e-03	kPa	369.50	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.05e-03	kPa	370.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	8.71e-04	kPa	370.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.18e-03	kPa	370.50	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.05e-03	kPa	371.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.29e-03	kPa	371.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.10e-03	kPa	371.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	

psub	9.77e-04	kPa	372.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.29e-03	kPa	373.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.38e-03	kPa	374.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.74e-03	kPa	374.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.35e-03	kPa	374.50	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.51e-03	kPa	375.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.86e-03	kPa	375.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.99e-03	kPa	375.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.66e-03	kPa	375.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.74e-03	kPa	376.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	2.29e-03	kPa	376.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.78e-03	kPa	376.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	

psub	1.48e-03	kPa	376.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.91e-03	kPa	377.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.70e-03	kPa	377.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	2.24e-03	kPa	378.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	2.46e-03	kPa	378.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	2.14e-03	kPa	378.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	2.24e-03	kPa	378.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	1.78e-03	kPa	378.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	2.69e-03	kPa	379.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	2.88e-03	kPa	379.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	2.63e-03	kPa	379.50	Thermal stability and related thermodynamic properties of N-ethylthiourea	
psub	2.95e-03	kPa	380.00	Thermal stability and related thermodynamic properties of N-ethylthiourea	

psub	2.19e-03	kPa	380.00	Thermal stability and related thermodynamic properties of N-ethylthiourea
psub	2.29e-03	kPa	380.50	Thermal stability and related thermodynamic properties of N-ethylthiourea

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

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
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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