2-Imidazolidinethione

Other names:

1,3-Ethylene-2-thiourea
1,3-Ethylenethiourea
2-Imidazoline-2-thiol
2-Imidozolidimethione
2-Mercapto-2-imidazoline
2-Mercaptoimidazoline
2-Thioimidazolidine
2-Thiol-dihydroglyoxaline
2-Thionoimidazolidine
2H-Imidazole-2-thione, tetrahydro-
4,5-Dihydro-2-mercaptoimidazole
4,5-Dihydroimidazole-2(3H)-thione
Akrochem ETU-22
Akroform ETU-22 PM
ETU
Ethylenethiourea
Imidazolidinethione
Imidazoline-2(3H)-Thione
Imidazoline-2-thiol
Mercaptoimidazoline
Mercazin I
Mercozen
N,N'-Ethylenethiourea
NA 22
NA-22-D
Nocceler 22
Pennac CRA
Perkacit ETU
Rhenogran ETU
Rhodanin S 62
Robac 22
Sanceller 22
Sodium-22 neoprene accelerator
Soxinol 22
Tetrahydro-2H-imidazole-2-thione
Thiourea, N,N'-(1,2-ethanediyl)-
Vulkacit NPV/C
Vulkacit NPV/C2
Warecure C
imidazolidine-2-thione

Inchi: InChI=1S/C3H6N2S/c6-3-4-1-2-5-3/h1-2H2,(H2,4,5,6)
InchiKey: PDQAZBWRQCGBEV-UHFFFAOYSA-N
Formula: C3H6N2S
SMILES: S=C1NCCN1
Mol. weight [g/mol]: 102.16
CAS: 96-45-7

Physical Properties

Property code	Value	Unit	Source
affp	921.90	kJ/mol	NIST Webbook
basg	891.20	kJ/mol	NIST Webbook
gf	284.91	kJ/mol	Joback Method
hf	166.29	kJ/mol	Joback Method
hfus	21.60	kJ/mol	Joback Method
hvap	43.83	kJ/mol	Joback Method
ie	8.15	eV	NIST Webbook
ie	8.15	eV	NIST Webbook
ie	8.15 ± 0.03	eV	NIST Webbook
log10ws	-0.71		Aqueous Solubility Prediction Method
logp	-0.536		Crippen Method
mcvol	74.280	ml/mol	McGowan Method
pc	7194.03	kPa	Joback Method
tb	457.73	K	Joback Method
tc	705.87	K	Joback Method
tf	412.44	K	Joback Method
vc	0.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	128.22	J/mol×K	457.73	Joback Method
cpg	136.75	J/mol×K	499.09	Joback Method
cpg	144.70	J/mol×K	540.44	Joback Method
cpg	152.12	J/mol×K	581.80	Joback Method
cpg	159.03	J/mol×K	623.16	Joback Method
cpg	165.47	J/mol×K	664.52	Joback Method

cpg	171.49	J/mol×K	705.87	Joback Method
hvapt	107.40	kJ/mol	298.15	Comprehensive Thermochemical Study of Cyclic Five- and Six-Membered N,N'-Thioureas

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96457&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Comprehensive Thermochemical Study of Cyclic Five- and Six-Membered N,N'-Thioureas:	https://www.doi.org/10.1021/acs.jced.7b00083
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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