Ethanedithioamide

Other names:	Dithiooxalic acid diamide
	Dithiooxamide
	Dithioxamide
	Hydrorubeanic acid
	NSC 1893
	Oxaldiimidic acid, dithio-
	Oxamide, dithio-
	RVK
	Rubean
	Rubeane
	Rubeanic acid
	USAF B-43
	USAF EK-4394
	USAF MK-6
Inchi:	InChI=1S/C2H4N2S2/c3-1(5)2(4)6/h(H2,3,5)(H2,4,6)
InchiKey:	OAEGRYMCJYIXQT-UHFFFAOYSA-N
Formula:	C2H4N2S2
SMILES:	NC(=S)C(N)=S
Mol. weight [g/mol]:	120.20
CAS:	79-40-3

Physical Properties

Property code	Value	Unit	Source
chs	-2541.90 ± 0.50	kJ/mol	NIST Webbook
gf	332.98	kJ/mol	Joback Method
hf	83.00 ± 1.50	kJ/mol	NIST Webbook
hfs	-20.80 ± 1.00	kJ/mol	NIST Webbook
hfus	20.54	kJ/mol	Joback Method
hsub	105.44	kJ/mol	NIST Webbook
hvap	54.79	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	-0.441		Crippen Method
mcvol	83.100	ml/mol	McGowan Method
pc	8087.06	kPa	Joback Method
tb	530.30	K	Joback Method
tc	794.73	K	Joback Method
tf	347.36	K	Joback Method

vc	0.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.90	J/mol×K	530.30	Joback Method
cpg	155.41	J/mol×K	574.37	Joback Method
cpg	159.27	J/mol×K	618.44	Joback Method
cpg	162.60	J/mol×K	662.52	Joback Method
cpg	165.53	J/mol×K	706.59	Joback Method
cpg	168.19	J/mol×K	750.66	Joback Method
cpg	170.70	J/mol×K	794.73	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.72578e+01
Coeff. B	-1.26988e+04
Temperature range (K), min.	470.84
Temperature range (K), max.	578.63

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C79403&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/54-584-4/Ethanedithioamide.pdf

Generated by Cheméo on 2024-10-12 04:08:26.754033217 +0000 UTC m=+3286969.391002466.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.