

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	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.72578e+01
Coeff. B	-1.26988e+04
Temperature range (K), min.	470.84
Temperature range (K), max.	578.63

Sources

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/ci9903071>

Crippen Method:

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

Joback Method:

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

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

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