Ethanediamide

Other names:	Amid kyseliny stavelove
	Diaminoglyoxal
	Formimidic acid, 1-carbamoyl-
	NH2COCONH2
	NSC 2770
	Oxalamide
	Oxalic acid diamide
	Oxamic acid amide
	Oxamid
	Oxamimidic acid
	ethanedioic acid, diamide
	oxamide
Inchi:	InChI=1S/C2H4N2O2/c3-1(5)2(4)6/h(H2,3,5)(H2,4,6)
InchiKey:	YIKSCQDJHCMVMK-UHFFFAOYSA-N
Formula:	C2H4N2O2
SMILES:	NC(=O)C(N)=O
Mol. weight [g/mol]:	88.07
CAS:	471-46-5

Physical Properties

Property code	Value	Unit	Source
chs	-853.43	kJ/mol	NIST Webbook
chs	-902.60	kJ/mol	NIST Webbook
chs	-854.30 ± 0.40	kJ/mol	NIST Webbook
chs	-843.10 ± 4.20	kJ/mol	NIST Webbook
gf	-158.98	kJ/mol	Joback Method
hf	-387.10 ± 1.30	kJ/mol	NIST Webbook
hfs	-504.40 ± 0.50	kJ/mol	NIST Webbook
hfs	-456.90	kJ/mol	NIST Webbook
hfs	-515.60 ± 4.20	kJ/mol	NIST Webbook
hfus	50.00	kJ/mol	Odd even effect in melting properties of 12 alkane-a,x-diamides
hsub	117.30 ± 1.20	kJ/mol	NIST Webbook
hsub	112.97	kJ/mol	NIST Webbook
hvap	54.82	kJ/mol	Joback Method
ie	9.80	eV	NIST Webbook

ie	9.80	eV	NIST Webbook
ie	9.41	eV	NIST Webbook
log10ws	0.92		Crippen Method
logp	-2.043		Crippen Method
mcvol	62.140	ml/mol	McGowan Method
pc	7305.14	kPa	Joback Method
ss	118.11	J/mol×K	NIST Webbook
tb	497.96	K	Joback Method
tc	723.03	K	Joback Method
tf	378.68	K	Joback Method
vc	0.217	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.14	J/mol×K	610.49	Joback Method
cpg	146.35	J/mol×K	648.01	Joback Method
cpg	150.26	J/mol×K	685.52	Joback Method
cpg	127.75	J/mol×K	497.96	Joback Method
cpg	132.85	J/mol×K	535.47	Joback Method
cpg	137.65	J/mol×K	572.98	Joback Method
cpg	153.90	J/mol×K	723.03	Joback Method
cps	113.89	J/mol×K	298.15	NIST Webbook
hsubt	115.80	kJ/mol	384.00	NIST Webbook
hsubt	113.00	kJ/mol	361.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Odd even effect in melting properties of 12 alkane-a,x-diamides:	https://www.doi.org/10.1016/j.jct.2006.04.004
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=C471465&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume