

Ethyl oxamate

Other names:	Oxamic acid ethyl ester Acetic acid, aminooxo-, ethyl ester Ethoxalamide Oxalic acid, monoethyl ester amide
Inchi:	InChI=1S/C4H7NO3/c1-2-8-4(7)3(5)6/h2H2,1H3,(H2,5,6)
InchiKey:	RZMZBHSKPLVQCP-UHFFFAOYSA-N
Formula:	C4H7NO3
SMILES:	CCOC(=O)C(N)=O
Mol. weight [g/mol]:	117.10
CAS:	617-36-7

Physical Properties

Property code	Value	Unit	Source
gf	-313.59	kJ/mol	Joback Method
hf	-449.48	kJ/mol	Joback Method
hfus	15.70	kJ/mol	Joback Method
hvap	51.04	kJ/mol	Joback Method
ie	9.85	eV	NIST Webbook
log10ws	0.43		Crippen Method
logp	-0.965		Crippen Method
mcvol	86.210	ml/mol	McGowan Method
pc	4849.43	kPa	Joback Method
tb	493.61	K	Joback Method
tc	698.85	K	Joback Method
tf	340.19	K	Joback Method
vc	0.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.43	J/molxK	493.61	Joback Method
cpg	189.82	J/molxK	527.82	Joback Method
cpg	196.90	J/molxK	562.02	Joback Method
cpg	203.67	J/molxK	596.23	Joback Method

cpg	210.13	J/mol×K	630.44	Joback Method
cpg	216.27	J/mol×K	664.64	Joback Method
cpg	222.08	J/mol×K	698.85	Joback Method

Sources

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=C617367&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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