

Acetaldoxime

Other names:	(E)-CH3CH=NOH Acetaldehyde oxime Acetaldoxime,syn & anti Aldoxime Ethanal oxime Ethylidenehydroxylamine USAF am-5 UN 2332
Inchi:	InChI=1S/C2H5NO/c1-2-3-4/h2,4H,1H3
InchiKey:	FZENGILVLUJGJX-UHFFFAOYSA-N
Formula:	C2H5NO
SMILES:	CC=NO
Mol. weight [g/mol]:	59.07
CAS:	107-29-9

Physical Properties

Property code	Value	Unit	Source
chl	-1430.01 ± 0.24	kJ/mol	NIST Webbook
chs	-1425.00	kJ/mol	NIST Webbook
hf	-22.55 ± 0.29	kJ/mol	NIST Webbook
hfl	-71.58 ± 0.28	kJ/mol	NIST Webbook
hfs	-85.80	kJ/mol	NIST Webbook
hvap	49.03 ± 0.07	kJ/mol	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	10.70 ± 0.20	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
log10ws	0.52		Crippen Method
logp	0.466		Crippen Method
mcvol	50.590	ml/mol	McGowan Method
pc	4938.44	kPa	Joback Method
rinpol	606.00		NIST Webbook
rinpol	606.00		NIST Webbook
ripol	1301.00		NIST Webbook
tb	388.20	K	NIST Webbook
tb	388.00	K	NIST Webbook
tb	387.15 ± 2.00	K	NIST Webbook
tc	599.91	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	241.10	J/mol×K	298.15	NIST Webbook
hvapt	48.00	kJ/mol	338.00	NIST Webbook

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=C107299&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

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