

# Propanedinitrile, (ethoxymethylene)-

<b>Other names:</b>	«alpha»-Cyano-«beta»-ethoxyacrylonitrile 2-Cyano-3-ethoxyacrylonitrile (Ethoxymethylene)malononitrile («beta»-Ethoxymethylene)malononitrile Malononitrile, (ethoxymethylene)- Ethoxymethylene malonitrile Ethoxymethylene-malonic acid dinitrile (Ethoxymethylene)propanedinitrile USAF A-9230 USAF KF-10 (beta-Ethoxymethylene)malononitrile alpha-Cyano-beta-ethoxyacrylonitrile 1,1-Dicyano-2-ethoxyethene 1-Ethoxy-2,2-dicyanoethene 2-Ethoxy-1,1-ethenedicarbonitrile NSC 27792 Propanedinitrile, 2-(ethoxymethylene)-
<b>Inchi:</b>	InChI=1S/C6H6N2O/c1-2-9-5-6(3-7)4-8/h5H,2H2,1H3
<b>InchiKey:</b>	OEICGMPRFOJHKO-UHFFFAOYSA-N
<b>Formula:</b>	C6H6N2O
<b>SMILES:</b>	CCOC=C(C#N)C#N
<b>Mol. weight [g/mol]:</b>	122.12
<b>CAS:</b>	123-06-8

## Physical Properties

Property code	Value	Unit	Source
gf	232.67	kJ/mol	Joback Method
hf	137.80	kJ/mol	Joback Method
hfus	14.39	kJ/mol	Joback Method
hvap	52.35	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	0.954		Crippen Method
mcvol	99.730	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
tb	567.30	K	Joback Method
tc	786.40	K	Joback Method
tf	290.55	K	Joback Method

vc

0.422

m<sup>3</sup>/kmol

Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.30	J/mol×K	567.30	Joback Method
cpg	215.26	J/mol×K	603.82	Joback Method
cpg	221.86	J/mol×K	640.33	Joback Method
cpg	228.09	J/mol×K	676.85	Joback Method
cpg	233.97	J/mol×K	713.37	Joback Method
cpg	239.52	J/mol×K	749.88	Joback Method
cpg	244.75	J/mol×K	786.40	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	433.20	K	1.60	NIST Webbook

## Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Joback Method:

[https://en.wikipedia.org/wiki/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=C123068&Units=SI>

## 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

<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log10 of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>t<sub>brp</sub>:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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