

# Ethyl(1,1-dimethylpropyl)malononitrile

**Inchi:** InChI=1S/C10H16N2/c1-5-9(3,4)10(6-2,7-11)8-12/h5-6H2,1-4H3  
**InchiKey:** PGJYGIZMFMZNAZ-UHFFFAOYSA-N  
**Formula:** C10H16N2  
**SMILES:** CCC(C)(C)C(C#N)(C#N)CC  
**Mol. weight [g/mol]:** 164.25  
**CAS:** 85688-95-5

## Physical Properties

Property code	Value	Unit	Source
chs	-6206.80 ± 1.70	kJ/mol	NIST Webbook
gf	305.36	kJ/mol	Joback Method
hf	61.30 ± 1.90	kJ/mol	NIST Webbook
hfs	-15.00 ± 1.70	kJ/mol	NIST Webbook
hfus	9.84	kJ/mol	Joback Method
hsub	76.30	kJ/mol	NIST Webbook
hsub	76.23 ± 0.75	kJ/mol	NIST Webbook
hsub	76.20 ± 0.80	kJ/mol	NIST Webbook
hvap	56.22	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.866		Crippen Method
mvol	154.520	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
tb	625.90	K	Joback Method
tc	844.90	K	Joback Method
tf	337.28	K	Joback Method
vc	0.625	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.24	J/mol×K	625.90	Joback Method
cpg	408.64	J/mol×K	662.40	Joback Method
cpg	420.17	J/mol×K	698.90	Joback Method
cpg	430.90	J/mol×K	735.40	Joback Method

cpg	440.89	J/mol×K	771.90	Joback Method
cpg	450.23	J/mol×K	808.40	Joback Method
cpg	458.97	J/mol×K	844.90	Joback Method
hfust	19.25	kJ/mol	307.50	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C85688955&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C85688955&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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