

# t-Butylmalononitrile

Inchi:	InChI=1S/C7H10N2/c1-7(2,3)6(4-8)5-9/h6H,1-3H3
InchiKey:	TUJPHMQZSDKRSL-UHFFFAOYSA-N
Formula:	C7H10N2
SMILES:	CC(C)(C)C(C#N)C#N
Mol. weight [g/mol]:	122.17
CAS:	4210-60-0

## Physical Properties

Property code	Value	Unit	Source
chs	-4250.61 ± 0.71	kJ/mol	NIST Webbook
gf	274.82	kJ/mol	Joback Method
hf	126.70 ± 0.54	kJ/mol	NIST Webbook
hfs	66.90 ± 0.71	kJ/mol	NIST Webbook
hfus	5.96	kJ/mol	Joback Method
hsub	59.80 ± 0.70	kJ/mol	NIST Webbook
hsub	59.83 ± 0.67	kJ/mol	NIST Webbook
hsub	59.80	kJ/mol	NIST Webbook
hvap	50.45	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.696		Crippen Method
mvol	112.250	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
tb	560.05	K	Joback Method
tc	782.47	K	Joback Method
tf	286.05	K	Joback Method
vc	0.463	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.27	J/mol×K	560.05	Joback Method
cpg	264.83	J/mol×K	597.12	Joback Method
cpg	273.73	J/mol×K	634.19	Joback Method
cpg	282.04	J/mol×K	671.26	Joback Method

cpg	289.77	J/mol×K	708.33	Joback Method
cpg	296.98	J/mol×K	745.40	Joback Method
cpg	303.70	J/mol×K	782.47	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4210600&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4210600&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>

## 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>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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