

# Tetraisobutylsuccinonitrile

**Inchi:** InChI=1S/C20H36N2/c1-15(2)9-19(13-21,10-16(3)4)20(14-22,11-17(5)6)12-18(7)8/h15-19  
**InchiKey:** KSZZCMITDIGDPJ-UHFFFAOYSA-N  
**Formula:** C20H36N2  
**SMILES:** CC(C)CC(C#N)(CC(C)C)C(C#N)(CC(C)C)CC(C)C  
**Mol. weight [g/mol]:** 304.51  
**CAS:** 85688-86-4

## Physical Properties

Property code	Value	Unit	Source
chs	-12750.70 ± 3.70	kJ/mol	NIST Webbook
gf	379.80	kJ/mol	Joback Method
hf	-111.70	kJ/mol	NIST Webbook
hfs	-264.40 ± 3.70	kJ/mol	NIST Webbook
hfus	21.65	kJ/mol	Joback Method
hsub	152.70	kJ/mol	NIST Webbook
hsub	152.70	kJ/mol	NIST Webbook
hvap	76.93	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	6.191		Crippen Method
mcvol	295.420	ml/mol	McGowan Method
pc	1028.60	kPa	Joback Method
tb	852.94	K	Joback Method
tc	1061.70	K	Joback Method
tf	389.98	K	Joback Method
vc	1.161	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.02	J/mol×K	852.94	Joback Method
cpg	960.17	J/mol×K	887.73	Joback Method
cpg	976.33	J/mol×K	922.53	Joback Method
cpg	991.58	J/mol×K	957.32	Joback Method
cpg	1006.02	J/mol×K	992.11	Joback Method

cpg	1019.74	J/mol×K	1026.91	Joback Method
cpg	1032.82	J/mol×K	1061.70	Joback Method
hfust	34.31	kJ/mol	360.20	NIST Webbook

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C85688864&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C85688864&amp;Units=SI</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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