

# Benzyliden-5,6,7,8-tetrahydronaphthyl-2-acetonitrile

<b>Inchi:</b>	InChI=1S/C19H17N/c20-14-19(12-15-6-2-1-3-7-15)18-11-10-16-8-4-5-9-17(16)13-18/h1-
<b>InchiKey:</b>	KWLAKAURBXFIEX-XDHOZWIPSA-N
<b>Formula:</b>	C19H17N
<b>SMILES:</b>	N#CC(=Cc1cccc1)c1ccc2c(c1)CCCC2
<b>Mol. weight [g/mol]:</b>	259.35
<b>CAS:</b>	21848-09-9

## Physical Properties

Property code	Value	Unit	Source
chs	-10165.00	kJ/mol	NIST Webbook
gf	575.87	kJ/mol	Joback Method
hf	373.92	kJ/mol	Joback Method
hfs	259.00	kJ/mol	NIST Webbook
hfus	27.63	kJ/mol	Joback Method
hvap	74.67	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.630		Crippen Method
mcvol	217.270	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
tb	819.24	K	Joback Method
tc	1082.88	K	Joback Method
tf	446.38	K	Joback Method
vc	0.841	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.30	J/mol×K	819.24	Joback Method
cpg	634.90	J/mol×K	863.18	Joback Method
cpg	649.35	J/mol×K	907.12	Joback Method
cpg	662.83	J/mol×K	951.06	Joback Method
cpg	675.51	J/mol×K	995.00	Joback Method
cpg	687.58	J/mol×K	1038.94	Joback Method
cpg	699.23	J/mol×K	1082.88	Joback Method

# 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=C21848099&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21848099&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>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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