

# 9-(Methylthio)nonanitrile

<b>Inchi:</b>	InChI=1S/C10H19NS/c1-12-10-8-6-4-2-3-5-7-9-11/h2-8,10H2,1H3
<b>InchiKey:</b>	KQKRRHTVZQEXBX-UHFFFAOYSA-N
<b>Formula:</b>	C10H19NS
<b>SMILES:</b>	CSCCCCCCCC#N
<b>Mol. weight [g/mol]:</b>	185.33
<b>CAS:</b>	58214-94-1

## Physical Properties

Property code	Value	Unit	Source
gf	199.62	kJ/mol	Joback Method
hf	-42.98	kJ/mol	Joback Method
hfus	27.29	kJ/mol	Joback Method
hvap	55.15	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.604		Crippen Method
mvol	169.490	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1637.50		NIST Webbook
tb	599.06	K	Joback Method
tc	797.23	K	Joback Method
tf	301.85	K	Joback Method
vc	0.675	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.13	J/mol×K	599.06	Joback Method
cpg	427.81	J/mol×K	632.09	Joback Method
cpg	440.82	J/mol×K	665.12	Joback Method
cpg	453.17	J/mol×K	698.15	Joback Method
cpg	464.88	J/mol×K	731.18	Joback Method
cpg	475.96	J/mol×K	764.20	Joback Method
cpg	486.43	J/mol×K	797.23	Joback Method

# Sources

<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=C58214941&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C58214941&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<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>hfus:</b>	Enthalpy of fusion at standard conditions
<b>h vap:</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>r in pol:</b>	Non-polar retention indices
<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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