

# 2-(Trifluoromethyl)phenyl acetonitrile

<b>Other names:</b>	o-Trifluoromethylphenylacetonitrile Benzeneacetonitrile, 2-(trifluoromethyl)-
<b>Inchi:</b>	InChI=1S/C9H6F3N/c10-9(11,12)8-4-2-1-3-7(8)5-6-13/h1-4H,5H2
<b>InchiKey:</b>	QXDCZSJGEUSERL-UHFFFAOYSA-N
<b>Formula:</b>	C9H6F3N
<b>SMILES:</b>	N#CCc1ccccc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	185.15
<b>CAS:</b>	3038-47-9

## Physical Properties

Property code	Value	Unit	Source
gf	-320.73	kJ/mol	Joback Method
hf	-436.23	kJ/mol	Joback Method
hfus	16.05	kJ/mol	Joback Method
hvap	45.30	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.771		Crippen Method
mvol	120.600	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
tb	533.64	K	Joback Method
tc	742.11	K	Joback Method
tf	299.31	K	Joback Method
vc	0.500	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.20	J/mol×K	533.64	Joback Method
cpg	282.50	J/mol×K	568.38	Joback Method
cpg	292.03	J/mol×K	603.13	Joback Method
cpg	300.84	J/mol×K	637.87	Joback Method
cpg	308.99	J/mol×K	672.62	Joback Method
cpg	316.51	J/mol×K	707.36	Joback Method
cpg	323.45	J/mol×K	742.11	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.00	K	1.50	NIST Webbook

## 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=C3038479&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3038479&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>

## 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>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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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