

# Benzamide, 2-trifluoromethyl-N-ethyl-N-nonyl-

<b>Inchi:</b>	InChI=1S/C19H28F3NO/c1-3-5-6-7-8-9-12-15-23(4-2)18(24)16-13-10-11-14-17(16)19(20)
<b>InchiKey:</b>	MCFWCYPISWQBQW-UHFFFAOYSA-N
<b>Formula:</b>	C19H28F3NO
<b>SMILES:</b>	CCCCCCCCCN(CC)C(=O)c1ccccc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	343.43

## Physical Properties

Property code	Value	Unit	Source
gf	-387.85	kJ/mol	Joback Method
hf	-852.56	kJ/mol	Joback Method
hfus	45.06	kJ/mol	Joback Method
hvap	65.87	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.918		Crippen Method
mvol	271.670	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinpol	2631.00		NIST Webbook
rinpol	2631.00		NIST Webbook
tb	726.67	K	Joback Method
tc	907.83	K	Joback Method
tf	429.42	K	Joback Method
vc	1.058	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.19	J/mol×K	726.67	Joback Method
cpg	821.24	J/mol×K	756.86	Joback Method
cpg	837.31	J/mol×K	787.06	Joback Method
cpg	852.46	J/mol×K	817.25	Joback Method
cpg	866.75	J/mol×K	847.44	Joback Method
cpg	880.23	J/mol×K	877.64	Joback Method
cpg	892.96	J/mol×K	907.83	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=U415608&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415608&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.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>rinpola:</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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