

# Benzamide, 2-(trifluoromethyl)-N-propyl-

<b>Inchi:</b>	InChI=1S/C11H12F3NO/c1-2-7-15-10(16)8-5-3-4-6-9(8)11(12,13)14/h3-6H,2,7H2,1H3,(H
<b>InchiKey:</b>	VLLYUSXCJYKKAB-UHFFFAOYSA-N
<b>Formula:</b>	C11H12F3NO
<b>SMILES:</b>	CCCNC(=O)c1ccccc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	231.21

## Physical Properties

Property code	Value	Unit	Source
gf	-476.60	kJ/mol	Joback Method
hf	-701.50	kJ/mol	Joback Method
hfus	26.42	kJ/mol	Joback Method
hvap	52.45	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.845		Crippen Method
mcvol	158.950	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1500.00		NIST Webbook
tb	581.36	K	Joback Method
tc	776.89	K	Joback Method
tf	359.45	K	Joback Method
vc	0.627	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.71	J/mol×K	581.36	Joback Method
cpg	411.80	J/mol×K	613.95	Joback Method
cpg	424.03	J/mol×K	646.54	Joback Method
cpg	435.45	J/mol×K	679.12	Joback Method
cpg	446.10	J/mol×K	711.71	Joback Method
cpg	456.03	J/mol×K	744.30	Joback Method
cpg	465.29	J/mol×K	776.89	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U407184&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407184&amp;Units=SI</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>hvp:</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>rinp:</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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