

# Benzamide, 3-(trifluoromethyl)-N-butyl-

<b>Inchi:</b>	InChI=1S/C12H14F3NO/c1-2-3-7-16-11(17)9-5-4-6-10(8-9)12(13,14)15/h4-6,8H,2-3,7H2
<b>InchiKey:</b>	CQSSXBUAUOOYFP-UHFFFAOYSA-N
<b>Formula:</b>	C12H14F3NO
<b>SMILES:</b>	CCCCNC(=O)c1cccc(C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	245.24

## Physical Properties

Property code	Value	Unit	Source
gf	-468.18	kJ/mol	Joback Method
hf	-722.14	kJ/mol	Joback Method
hfus	29.01	kJ/mol	Joback Method
hvap	54.68	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.235		Crippen Method
mcvol	173.040	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
tb	604.24	K	Joback Method
tc	797.30	K	Joback Method
tf	370.72	K	Joback Method
vc	0.683	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.25	J/mol×K	604.24	Joback Method
cpg	460.91	J/mol×K	636.42	Joback Method
cpg	473.69	J/mol×K	668.59	Joback Method
cpg	485.65	J/mol×K	700.77	Joback Method
cpg	496.84	J/mol×K	732.95	Joback Method
cpg	507.28	J/mol×K	765.13	Joback Method
cpg	517.04	J/mol×K	797.30	Joback Method

# Sources

<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=U407167&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407167&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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