

# Benzamide, 4-(trifluoromethyl)-N-pentyl-

<b>Inchi:</b>	InChI=1S/C13H16F3NO/c1-2-3-4-9-17-12(18)10-5-7-11(8-6-10)13(14,15)16/h5-8H,2-4,9
<b>InchiKey:</b>	FRWVLNLLKLPARA-UHFFFAOYSA-N
<b>Formula:</b>	C13H16F3NO
<b>SMILES:</b>	CCCCCNC(=O)c1ccc(C(F)(F)F)cc1
<b>Mol. weight [g/mol]:</b>	259.27

## Physical Properties

Property code	Value	Unit	Source
gf	-459.76	kJ/mol	Joback Method
hf	-742.78	kJ/mol	Joback Method
hfus	31.60	kJ/mol	Joback Method
hvap	56.91	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.625		Crippen Method
mcvol	187.130	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
tb	627.12	K	Joback Method
tc	817.97	K	Joback Method
tf	381.99	K	Joback Method
vc	0.740	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.26	J/molxK	627.12	Joback Method
cpg	511.41	J/molxK	658.93	Joback Method
cpg	524.69	J/molxK	690.74	Joback Method
cpg	537.13	J/molxK	722.55	Joback Method
cpg	548.77	J/molxK	754.36	Joback Method
cpg	559.68	J/molxK	786.16	Joback Method
cpg	569.88	J/molxK	817.97	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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=U407299&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407299&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>

# 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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