

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

<b>Inchi:</b>	InChI=1S/C12H14F3NO/c1-8(2)7-16-11(17)9-3-5-10(6-4-9)12(13,14)15/h3-6,8H,7H2,1-2
<b>InchiKey:</b>	MVNNWOBVCNJDSA-UHFFFAOYSA-N
<b>Formula:</b>	C12H14F3NO
<b>SMILES:</b>	CC(C)CNC(=O)c1ccc(C(F)(F)F)cc1
<b>Mol. weight [g/mol]:</b>	245.24

## Physical Properties

Property code	Value	Unit	Source
gf	-470.62	kJ/mol	Joback Method
hf	-727.42	kJ/mol	Joback Method
hfus	25.49	kJ/mol	Joback Method
hvap	54.29	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.091		Crippen Method
mvol	173.040	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	1571.00		NIST Webbook
rinpol	1571.00		NIST Webbook
tb	603.80	K	Joback Method
tc	800.52	K	Joback Method
tf	355.72	K	Joback Method
vc	0.677	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.67	J/molxK	603.80	Joback Method
cpg	461.64	J/molxK	636.59	Joback Method
cpg	474.69	J/molxK	669.37	Joback Method
cpg	486.88	J/molxK	702.16	Joback Method
cpg	498.25	J/molxK	734.95	Joback Method
cpg	508.85	J/molxK	767.74	Joback Method
cpg	518.73	J/molxK	800.52	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U407296&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407296&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.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>

# 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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