

# Benzamide, 2-trifluoromethyl-N-ethyl-N-3-methylbutyl-

<b>Inchi:</b>	InChI=1S/C15H20F3NO/c1-4-19(10-9-11(2)3)14(20)12-7-5-6-8-13(12)15(16,17)18/h5-8,
<b>InchiKey:</b>	KPGLXXKPPQNVCD-UHFFFAOYSA-N
<b>Formula:</b>	C15H20F3NO
<b>SMILES:</b>	CCN(CCC(C)C)C(=O)c1ccccc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	287.32

## Physical Properties

Property code	Value	Unit	Source
gf	-423.97	kJ/mol	Joback Method
hf	-775.28	kJ/mol	Joback Method
hfus	31.18	kJ/mol	Joback Method
hvap	56.58	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.214		Crippen Method
mvol	215.310	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	1912.00		NIST Webbook
rinpol	1912.00		NIST Webbook
tb	634.71	K	Joback Method
tc	821.77	K	Joback Method
tf	369.34	K	Joback Method
vc	0.829	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.31	J/mol×K	634.71	Joback Method
cpg	600.43	J/mol×K	665.89	Joback Method
cpg	615.56	J/mol×K	697.06	Joback Method
cpg	629.76	J/mol×K	728.24	Joback Method
cpg	643.08	J/mol×K	759.42	Joback Method
cpg	655.58	J/mol×K	790.59	Joback Method
cpg	667.29	J/mol×K	821.77	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=U415602&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415602&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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