

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

Inchi:	InChI=1S/C10H9F4NO/c1-2-15-9(16)6-4-3-5-7(8(6)11)10(12,13)14/h3-5H,2H2,1H3,(H,15)
InchiKey:	LXBHPXKKBR CXBO-UHFFFAOYSA-N
Formula:	C10H9F4NO
SMILES:	CCNC(=O)c1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]:	235.18

## Physical Properties

Property code	Value	Unit	Source
gf	-689.46	kJ/mol	Joback Method
hf	-888.44	kJ/mol	Joback Method
hfus	26.52	kJ/mol	Joback Method
hvap	50.07	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.594		Crippen Method
mcvol	146.630	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	1305.00		NIST Webbook
tb	562.73	K	Joback Method
tc	752.89	K	Joback Method
tf	361.29	K	Joback Method
vc	0.590	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.53	J/molxK	562.73	Joback Method
cpg	371.10	J/molxK	594.42	Joback Method
cpg	381.94	J/molxK	626.12	Joback Method
cpg	392.07	J/molxK	657.81	Joback Method
cpg	401.54	J/molxK	689.50	Joback Method
cpg	410.38	J/molxK	721.20	Joback Method
cpg	418.63	J/molxK	752.89	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=U407698&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407698&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>rinpol:</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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