

# Benzamide, 3-fluoro-5-trifluoromethyl-N-(3-fluoro-5-trifluoromethyl)

**Inchi:** InChI=1S/C30H35F8NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-39(27(40)21-17-22(29(33,34)35)36)37-38  
**InchiKey:** IEFHXGVVVDXVDP-UHFFFAOYSA-N  
**Formula:** C30H35F8NO2  
**SMILES:** CCCCCCCCCCCCCCN(C(=O)c1cc(F)cc(C(F)(F)F)c1)C(=O)c1cc(F)ccc1C(F)(F)F  
**Mol. weight [g/mol]:** 593.59

## Physical Properties

Property code	Value	Unit	Source
gf	-1311.84	kJ/mol	Joback Method
hf	-1979.36	kJ/mol	Joback Method
hfus	76.01	kJ/mol	Joback Method
hvap	95.98	kJ/mol	Joback Method
log10ws	-11.89		Crippen Method
logp	9.986		Crippen Method
mvol	413.320	ml/mol	McGowan Method
pc	732.84	kPa	Joback Method
rinpol	2649.00		NIST Webbook
rinpol	2649.00		NIST Webbook
tb	1066.96	K	Joback Method
tc	1324.97	K	Joback Method
tf	672.67	K	Joback Method
vc	1.651	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1423.91	J/molxK	1066.96	Joback Method
cpg	1441.85	J/molxK	1109.96	Joback Method
cpg	1458.78	J/molxK	1152.96	Joback Method
cpg	1474.96	J/molxK	1195.96	Joback Method
cpg	1490.62	J/molxK	1238.97	Joback Method
cpg	1506.01	J/molxK	1281.97	Joback Method
cpg	1521.36	J/molxK	1324.97	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=U407881&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407881&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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