

# Benzamide, 3-trifluoromethyl-2-fluoro-N-(3-trifluoromethyl-2-fluorophenyl)-

Inchi:	InChI=1S/C21H17F8NO2/c1-2-3-4-11-30(18(31)12-7-5-9-14(16(12)22)20(24,25)26)19(32)33
InchiKey:	ZNNXVRPDATVDRD-UHFFFAOYSA-N
Formula:	C21H17F8NO2
SMILES:	CCCCCN(C(=O)c1cccc(C(F)(F)F)c1F)C(=O)c1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]:	467.35

## Physical Properties

Property code	Value	Unit	Source
gf	-1387.62	kJ/mol	Joback Method
hf	-1793.60	kJ/mol	Joback Method
hfus	52.70	kJ/mol	Joback Method
hvap	75.95	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	6.475		Crippen Method
mvol	286.510	ml/mol	McGowan Method
pc	1248.61	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	861.04	K	Joback Method
tc	1059.25	K	Joback Method
tf	571.24	K	Joback Method
vc	1.147	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.19	J/molxK	861.04	Joback Method
cpg	895.38	J/molxK	894.08	Joback Method
cpg	906.72	J/molxK	927.11	Joback Method
cpg	917.27	J/molxK	960.15	Joback Method
cpg	927.14	J/molxK	993.18	Joback Method
cpg	936.40	J/molxK	1026.22	Joback Method
cpg	945.14	J/molxK	1059.25	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U407722&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407722&amp;Units=SI</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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