

# 3-Fluoro-6-trifluoromethylbenzamide, N-(4-bromophenyl)-

<b>Inchi:</b>	InChI=1S/C14H8BrF4NO/c15-8-1-4-10(5-2-8)20-13(21)11-7-9(16)3-6-12(11)14(17,18)19
<b>InchiKey:</b>	DWRZGTBIEFFRQQ-UHFFFAOYSA-N
<b>Formula:</b>	C14H8BrF4NO
<b>SMILES:</b>	O=C(Nc1ccc(Br)cc1)c1cc(F)ccc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	362.12

## Physical Properties

Property code	Value	Unit	Source
gf	-538.68	kJ/mol	Joback Method
hf	-719.61	kJ/mol	Joback Method
hfus	35.82	kJ/mol	Joback Method
hvap	68.35	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	4.859		Crippen Method
mcvol	196.730	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	2164.00		NIST Webbook
rinpol	2164.00		NIST Webbook
tb	752.07	K	Joback Method
tc	979.70	K	Joback Method
tf	505.11	K	Joback Method
vc	0.767	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.60	J/mol×K	752.07	Joback Method
cpg	516.12	J/mol×K	790.01	Joback Method
cpg	525.73	J/mol×K	827.95	Joback Method
cpg	534.51	J/mol×K	865.88	Joback Method
cpg	542.54	J/mol×K	903.82	Joback Method
cpg	549.92	J/mol×K	941.76	Joback Method
cpg	556.72	J/mol×K	979.70	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=U358084&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358084&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>

# 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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