

# 3-Fluoro-6-trifluoromethylbenzamide, N-(2-octyl)-

**Inchi:** InChI=1S/C16H21F4NO/c1-3-4-5-6-7-11(2)21-15(22)13-10-12(17)8-9-14(13)16(18,19)20  
**InchiKey:** LMVQLZYGOUYUFD-UHFFFAOYSA-N  
**Formula:** C16H21F4NO  
**SMILES:** CCCCCC(C)NC(=O)c1cc(F)ccc1C(F)(F)F  
**Mol. weight [g/mol]:** 319.34

## Physical Properties

Property code	Value	Unit	Source
gf	-641.38	kJ/mol	Joback Method
hf	-1017.56	kJ/mol	Joback Method
hfus	38.54	kJ/mol	Joback Method
hvap	63.04	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	4.933		Crippen Method
mvol	231.170	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	1833.00		NIST Webbook
rinpol	1833.00		NIST Webbook
tb	699.57	K	Joback Method
tc	883.23	K	Joback Method
tf	413.91	K	Joback Method
vc	0.919	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.14	J/mol×K	699.57	Joback Method
cpg	678.04	J/mol×K	730.18	Joback Method
cpg	692.06	J/mol×K	760.79	Joback Method
cpg	705.25	J/mol×K	791.40	Joback Method
cpg	717.65	J/mol×K	822.01	Joback Method
cpg	729.30	J/mol×K	852.62	Joback Method
cpg	740.26	J/mol×K	883.23	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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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=U358076&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358076&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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