

# 3-Fluoro-6-trifluoromethylbenzamide, N,N-di(2-ethylhexyl)-

<b>Inchi:</b>	InChI=1S/C24H37F4NO/c1-5-9-11-18(7-3)16-29(17-19(8-4)12-10-6-2)23(30)21-15-20(25
<b>InchiKey:</b>	AZKKDGMWSBOOPB-UHFFFAOYSA-N
<b>Formula:</b>	C24H37F4NO
<b>SMILES:</b>	CCCCC(CC)CN(CC(CC)CCCC)C(=O)c1cc(F)ccc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	431.55

## Physical Properties

Property code	Value	Unit	Source
gf	-555.07	kJ/mol	Joback Method
hf	-1173.90	kJ/mol	Joback Method
hfus	53.66	kJ/mol	Joback Method
hvap	76.07	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	7.720		Crippen Method
mcvol	343.890	ml/mol	McGowan Method
pc	915.50	kPa	Joback Method
rinsol	2275.00		NIST Webbook
tb	844.44	K	Joback Method
tc	1035.03	K	Joback Method
tf	468.88	K	Joback Method
vc	1.345	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1109.87	J/molxK	844.44	Joback Method
cpg	1128.38	J/molxK	876.21	Joback Method
cpg	1145.80	J/molxK	907.97	Joback Method
cpg	1162.20	J/molxK	939.74	Joback Method
cpg	1177.66	J/molxK	971.50	Joback Method
cpg	1192.24	J/molxK	1003.27	Joback Method
cpg	1206.02	J/molxK	1035.03	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=U358082&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358082&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>
<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>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>mccvol:</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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