

# Benzamide, 3-fluoro-5-trifluoromethyl-N-heptyl-

Inchi:	InChI=1S/C15H19F4NO/c1-2-3-4-5-6-7-20-14(21)11-8-12(15(17,18)19)10-13(16)9-11/h8
InchiKey:	ZHJQRAHMMJXGRF-UHFFFAOYSA-N
Formula:	C15H19F4NO
SMILES:	CCCCCCCNC(=O)c1cc(F)cc(C(F)(F)F)c1
Mol. weight [g/mol]:	305.31

## Physical Properties

Property code	Value	Unit	Source
gf	-647.36	kJ/mol	Joback Method
hf	-991.64	kJ/mol	Joback Method
hfus	39.47	kJ/mol	Joback Method
hvap	61.20	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.545		Crippen Method
mcvol	217.080	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpola	1815.00		NIST Webbook
rinpola	1815.00		NIST Webbook
tb	677.13	K	Joback Method
tc	859.00	K	Joback Method
tf	417.64	K	Joback Method
vc	0.870	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.77	J/mol×K	677.13	Joback Method
cpg	623.05	J/mol×K	707.44	Joback Method
cpg	636.50	J/mol×K	737.75	Joback Method
cpg	649.16	J/mol×K	768.06	Joback Method
cpg	661.07	J/mol×K	798.38	Joback Method
cpg	672.28	J/mol×K	828.69	Joback Method
cpg	682.82	J/mol×K	859.00	Joback Method

# Sources

<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=U407857&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407857&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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