

# Benzamide, 3-fluoro-N-butyl-N-hept-2-yl-

<b>Inchi:</b>	InChI=1S/C18H28FNO/c1-4-6-8-10-15(3)20(13-7-5-2)18(21)16-11-9-12-17(19)14-16/h9,
<b>InchiKey:</b>	JMSFUHWYRKFTKX-UHFFFAOYSA-N
<b>Formula:</b>	C18H28FNO
<b>SMILES:</b>	CCCCC(C)N(CCCC)C(=O)c1cccc(F)c1
<b>Mol. weight [g/mol]:</b>	293.42

## Physical Properties

Property code	Value	Unit	Source
gf	-11.93	kJ/mol	Joback Method
hf	-436.23	kJ/mol	Joback Method
hfus	40.20	kJ/mol	Joback Method
hvap	66.18	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.037		Crippen Method
mvol	254.040	ml/mol	McGowan Method
pc	1472.49	kPa	Joback Method
rinpol	2363.00		NIST Webbook
rinpol	2363.00		NIST Webbook
tb	708.04	K	Joback Method
tc	896.39	K	Joback Method
tf	399.55	K	Joback Method
vc	0.972	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.17	J/mol×K	708.04	Joback Method
cpg	747.95	J/mol×K	739.43	Joback Method
cpg	764.73	J/mol×K	770.82	Joback Method
cpg	780.55	J/mol×K	802.22	Joback Method
cpg	795.46	J/mol×K	833.61	Joback Method
cpg	809.50	J/mol×K	865.00	Joback Method
cpg	822.72	J/mol×K	896.39	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U415865&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415865&amp;Units=SI</a>
<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>

# 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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