

# Benzamide, 3-fluoro-N-(hept-2-yl)-

<b>Inchi:</b>	InChI=1S/C14H20FNO/c1-3-4-5-7-11(2)16-14(17)12-8-6-9-13(15)10-12/h6,8-11H,3-5,7H
<b>InchiKey:</b>	PMEJQPYJOPSJBY-UHFFFAOYSA-N
<b>Formula:</b>	C14H20FNO
<b>SMILES:</b>	CCCCC(C)NC(=O)c1cccc(F)c1
<b>Mol. weight [g/mol]:</b>	237.31

## Physical Properties

Property code	Value	Unit	Source
gf	-67.00	kJ/mol	Joback Method
hf	-367.73	kJ/mol	Joback Method
hfus	31.92	kJ/mol	Joback Method
hvap	61.67	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.524		Crippen Method
mvol	197.680	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1809.00		NIST Webbook
rinpol	1809.00		NIST Webbook
tb	654.25	K	Joback Method
tc	852.57	K	Joback Method
tf	374.66	K	Joback Method
vc	0.764	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.21	J/mol×K	654.25	Joback Method
cpg	545.84	J/mol×K	687.30	Joback Method
cpg	560.55	J/mol×K	720.36	Joback Method
cpg	574.39	J/mol×K	753.41	Joback Method
cpg	587.39	J/mol×K	786.46	Joback Method
cpg	599.59	J/mol×K	819.51	Joback Method
cpg	611.02	J/mol×K	852.57	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.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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U407281&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407281&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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