

# 3-Chloro-2-fluorobenzamide, N-(2-octyl)-

<b>Inchi:</b>	InChI=1S/C15H21ClFNO/c1-3-4-5-6-8-11(2)18-15(19)12-9-7-10-13(16)14(12)17/h7,9-11
<b>InchiKey:</b>	BBPNKNMZAYDYKS-UHFFFAOYSA-N
<b>Formula:</b>	C15H21ClFNO
<b>SMILES:</b>	CCCCCCC(C)NC(=O)c1cccc(Cl)c1F
<b>Mol. weight [g/mol]:</b>	285.79

## Physical Properties

Property code	Value	Unit	Source
gf	-80.14	kJ/mol	Joback Method
hf	-415.58	kJ/mol	Joback Method
hfus	38.32	kJ/mol	Joback Method
hvap	68.95	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.568		Crippen Method
mcvol	224.010	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinsol	2059.00		NIST Webbook
tb	719.54	K	Joback Method
tc	920.23	K	Joback Method
tf	428.37	K	Joback Method
vc	0.870	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.41	J/mol×K	719.54	Joback Method
cpg	626.24	J/mol×K	752.99	Joback Method
cpg	640.18	J/mol×K	786.44	Joback Method
cpg	653.26	J/mol×K	819.89	Joback Method
cpg	665.51	J/mol×K	853.33	Joback Method
cpg	676.97	J/mol×K	886.78	Joback Method
cpg	687.68	J/mol×K	920.23	Joback Method

# Sources

<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>
<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=U358132&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358132&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>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>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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