

# Benzamide, 3-chloro-2-fluoro-N-tetradecyl-

<b>Inchi:</b>	InChI=1S/C21H33ClFNO/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-24-21(25)18-15-14-16-19(2)
<b>InchiKey:</b>	GSHQDUXVHZMJFI-UHFFFAOYSA-N
<b>Formula:</b>	C21H33ClFNO
<b>SMILES:</b>	CCCCCCCCCCCCNC(=O)c1cccc(Cl)c1F
<b>Mol. weight [g/mol]:</b>	369.94

## Physical Properties

Property code	Value	Unit	Source
gf	-27.18	kJ/mol	Joback Method
hf	-534.14	kJ/mol	Joback Method
hfus	57.38	kJ/mol	Joback Method
hvap	82.69	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	6.910		Crippen Method
mvol	308.550	ml/mol	McGowan Method
pc	1157.71	kPa	Joback Method
rinpol	2822.00		NIST Webbook
rinpol	2822.00		NIST Webbook
tb	857.26	K	Joback Method
tc	1055.17	K	Joback Method
tf	510.99	K	Joback Method
vc	1.212	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.47	J/mol×K	857.26	Joback Method
cpg	971.10	J/mol×K	890.25	Joback Method
cpg	986.71	J/mol×K	923.23	Joback Method
cpg	1001.35	J/mol×K	956.22	Joback Method
cpg	1015.08	J/mol×K	989.20	Joback Method
cpg	1027.94	J/mol×K	1022.19	Joback Method
cpg	1039.98	J/mol×K	1055.17	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=U407832&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U407832&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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