

# Benzoic acid, 4-[3-(2-chloroethyl)ureido]-3,5-dimethyl-

Inchi:	InChI=1S/C12H15ClN2O3/c1-7-5-9(11(16)17)6-8(2)10(7)15-12(18)14-4-3-13/h5-6H,3-4H
InchiKey:	VFKPCRRWRRRCZNL-UHFFFAOYSA-N
Formula:	C12H15ClN2O3
SMILES:	<chem>Cc1cc(C(=O)O)cc(C)c1NC(=O)NCCCl</chem>
Mol. weight [g/mol]:	270.71
CAS:	116465-96-4

## Physical Properties

Property code	Value	Unit	Source
gf	-94.13	kJ/mol	Joback Method
hf	-375.08	kJ/mol	Joback Method
hfus	41.39	kJ/mol	Joback Method
hvap	94.00	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.362		Crippen Method
mcvol	197.390	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
tb	853.27	K	Joback Method
tc	1064.45	K	Joback Method
tf	584.90	K	Joback Method
vc	0.750	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.81	J/molxK	853.27	Joback Method
cpg	564.25	J/molxK	888.47	Joback Method
cpg	572.98	J/molxK	923.66	Joback Method
cpg	581.00	J/molxK	958.86	Joback Method
cpg	588.35	J/molxK	994.06	Joback Method
cpg	595.07	J/molxK	1029.26	Joback Method
cpg	601.17	J/molxK	1064.45	Joback Method

# Sources

<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=C116465964&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116465964&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>
<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>

# 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>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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