

Benzamide, 2-chloro-N-methyl-

Inchi:	InChI=1S/C8H8ClNO/c1-10-8(11)6-4-2-3-5-7(6)9/h2-5H,1H3,(H,10,11)
InchiKey:	ITXNDDPDABTCBO-UHFFFAOYSA-N
Formula:	C8H8ClNO
SMILES:	CN=C(O)c1ccccc1Cl
Mol. weight [g/mol]:	169.61

Physical Properties

Property code	Value	Unit	Source
hf	-78.93	kJ/mol	Joback Method
hvap	60.80	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.274		Crippen Method
mcvol	123.610	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
rinsol	1527.00		NIST Webbook
rinsol	1527.00		NIST Webbook
tb	620.27	K	Joback Method
tc	843.37	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407426&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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