

Benzamide, 3-chloro-N-butyl-

Inchi:	InChI=1S/C11H14ClNO/c1-2-3-7-13-11(14)9-5-4-6-10(12)8-9/h4-6,8H,2-3,7H2,1H3,(H,1
InchiKey:	NKQOQWJDLCYELT-UHFFFAOYSA-N
Formula:	C11H14ClNO
SMILES:	CCCCN=C(O)c1cccc(Cl)c1
Mol. weight [g/mol]:	211.69

Physical Properties

Property code	Value	Unit	Source
hf	-140.85	kJ/mol	Joback Method
hvap	67.48	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.445		Crippen Method
mcpvol	165.880	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1850.00		NIST Webbook
rinpol	1850.00		NIST Webbook
tb	688.91	K	Joback Method
tc	901.01	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U407975&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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<https://www.chemeo.com/cid/95-150-0/Benzamide-3-chloro-N-butyl.pdf>

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