

Benzamide, 3-chloro-N-ethyl-

Inchi:	InChI=1S/C9H10ClNO/c1-2-11-9(12)7-4-3-5-8(10)6-7/h3-6H,2H2,1H3,(H,11,12)
InchiKey:	FOUXUKUHVUPLEP-UHFFFAOYSA-N
Formula:	C9H10ClNO
SMILES:	CCN=C(O)c1cccc(Cl)c1
Mol. weight [g/mol]:	183.63

Physical Properties

Property code	Value	Unit	Source
hf	-99.57	kJ/mol	Joback Method
hvap	63.02	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.665		Crippen Method
mcvol	137.700	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	1648.00		NIST Webbook
rinpol	1648.00		NIST Webbook
tb	643.15	K	Joback Method
tc	862.26	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407972&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

Latest version available from:

<https://www.cheméo.com/cid/97-128-3/Benzamide-3-chloro-N-ethyl.pdf>

Generated by Cheméo on 2024-04-27 15:11:46.927505054 +0000 UTC m=+16519955.848082369.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.