

Benzamide, 3-chloro-N-pentyl-

Inchi:	InChI=1S/C12H16ClNO/c1-2-3-4-8-14-12(15)10-6-5-7-11(13)9-10/h5-7,9H,2-4,8H2,1H3,
InchiKey:	OWIOHGXMJPRXCO-UHFFFAOYSA-N
Formula:	C12H16ClNO
SMILES:	CCCCCN=C(O)c1cccc(Cl)c1
Mol. weight [g/mol]:	225.72

Physical Properties

Property code	Value	Unit	Source
hf	-161.49	kJ/mol	Joback Method
hvap	69.70	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.835		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
rinpol	1948.00		NIST Webbook
rinpol	1948.00		NIST Webbook
tb	711.79	K	Joback Method
tc	920.97	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407977&Units=SI
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

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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