

Benzamide, 2-chloro-N-undecyl-

Inchi:	InChI=1S/C18H28ClNO/c1-2-3-4-5-6-7-8-9-12-15-20-18(21)16-13-10-11-14-17(16)19/h1
InchiKey:	DEBKRCDZDHPIGM-UHFFFAOYSA-N
Formula:	C18H28ClNO
SMILES:	CCCCCCCCCCCN=C(O)c1cccc1Cl
Mol. weight [g/mol]:	309.87

Physical Properties

Property code	Value	Unit	Source
hf	-285.33	kJ/mol	Joback Method
hvap	83.06	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	6.175		Crippen Method
mcvol	264.510	ml/mol	McGowan Method
pc	1397.50	kPa	Joback Method
rinpol	2533.00		NIST Webbook
rinpol	2533.00		NIST Webbook
tb	849.07	K	Joback Method
tc	1051.41	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407439&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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