

Benzamide, 3-methyl-N-dodecyl-

Inchi:	InChI=1S/C20H33NO/c1-3-4-5-6-7-8-9-10-11-12-16-21-20(22)19-15-13-14-18(2)17-19/h
InchiKey:	TXYLMETUSBLFMP-UHFFFAOYSA-N
Formula:	C20H33NO
SMILES:	CCCCCCCCCCCN=C(O)c1cccc(C)c1
Mol. weight [g/mol]:	303.48

Physical Properties

Property code	Value	Unit	Source
hf	-310.87	kJ/mol	Joback Method
hvap	83.12	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	6.221		Crippen Method
mcvol	280.450	ml/mol	McGowan Method
pc	1248.61	kPa	Joback Method
rinpol	2609.00		NIST Webbook
rinpol	2609.00		NIST Webbook
tb	857.40	K	Joback Method
tc	1056.73	K	Joback Method

Sources

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=U407422&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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