

Benzamide, 4-hydroxy, 3-(1-methylethyl), N-methyl

Inchi:	InChI=1S/C11H15NO2/c1-7(2)9-6-8(11(14)12-3)4-5-10(9)13/h4-7,13H,1-3H3,(H,12,14)
InchiKey:	VHSHBXVHECBNDY-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	CN=C(O)c1ccc(O)c(C(C)C)c1
Mol. weight [g/mol]:	193.24

Physical Properties

Property code	Value	Unit	Source
hf	-307.70	kJ/mol	Joback Method
hvap	75.72	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.450		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinpol	1837.00		NIST Webbook
rinpol	1837.00		NIST Webbook
tb	731.66	K	Joback Method
tc	952.73	K	Joback Method

Sources

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=R84552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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