

Benzamide, 2-methyl-N-isobutyl-

Inchi:	InChI=1S/C12H17NO/c1-9(2)8-13-12(14)11-7-5-4-6-10(11)3/h4-7,9H,8H2,1-3H3,(H,13,1
InchiKey:	MXGMXFIGOFJSMS-UHFFFAOYSA-N
Formula:	C12H17NO
SMILES:	Cc1ccccc1C(O)=NCC(C)C
Mol. weight [g/mol]:	191.27

Physical Properties

Property code	Value	Unit	Source
hf	-151.03	kJ/mol	Joback Method
hvap	64.93	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.956		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
rinsol	1652.00		NIST Webbook
tb	673.92	K	Joback Method
tc	883.38	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U407393&Units=SI

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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