

Benzamide, 2-methyl-N-propyl-

Inchi:	InChI=1S/C11H15NO/c1-3-8-12-11(13)10-7-5-4-6-9(10)2/h4-7H,3,8H2,1-2H3,(H,12,13)
InchiKey:	GYZQPZPWICRXQY-UHFFFAOYSA-N
Formula:	C11H15NO
SMILES:	CCCN=C(O)c1ccccc1C
Mol. weight [g/mol]:	177.24

Physical Properties

Property code	Value	Unit	Source
hf	-125.11	kJ/mol	Joback Method
hvap	63.09	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.710		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
tb	651.48	K	Joback Method
tc	860.19	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=U407392&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
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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