

Benzamide, 3-methoxy-N-propyl-

Inchi:	InChI=1S/C11H15NO2/c1-3-7-12-11(13)9-5-4-6-10(8-9)14-2/h4-6,8H,3,7H2,1-2H3,(H,12
InchiKey:	XOKXCBFLSDEEIB-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	CCCN=C(O)c1cccc(OC)c1
Mol. weight [g/mol]:	193.24

Physical Properties

Property code	Value	Unit	Source
hf	-257.33	kJ/mol	Joback Method
hvap	65.50	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.410		Crippen Method
mcpvol	159.510	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	1803.00		NIST Webbook
rinpol	1803.00		NIST Webbook
tb	673.90	K	Joback Method
tc	880.60	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407507&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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