

Benzamide, 3-methyl-N-ethyl-

Inchi:	InChI=1S/C10H13NO/c1-3-11-10(12)9-6-4-5-8(2)7-9/h4-7H,3H2,1-2H3,(H,11,12)
InchiKey:	FPINATACRXASTP-UHFFFAOYSA-N
Formula:	C10H13NO
SMILES:	CCN=C(O)c1cccc(C)c1
Mol. weight [g/mol]:	163.22

Physical Properties

Property code	Value	Unit	Source
hf	-104.47	kJ/mol	Joback Method
hvap	60.87	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.320		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1572.00		NIST Webbook
tb	628.60	K	Joback Method
tc	840.60	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407408&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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