

Benzamide, 3-fluoro-N-isobutyl-

Inchi:	InChI=1S/C11H14FNO/c1-8(2)7-13-11(14)9-4-3-5-10(12)6-9/h3-6,8H,7H2,1-2H3,(H,13,1
InchiKey:	GWVXRPGYQSFSML-UHFFFAOYSA-N
Formula:	C11H14FNO
SMILES:	CC(C)CN=C(O)c1cccc(F)c1
Mol. weight [g/mol]:	195.23

Physical Properties

Property code	Value	Unit	Source
hf	-326.50	kJ/mol	Joback Method
hvap	61.89	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.786		Crippen Method
mcvol	155.410	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1582.00		NIST Webbook
rinpol	1582.00		NIST Webbook
tb	650.31	K	Joback Method
tc	854.00	K	Joback Method

Sources

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=U407277&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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