

Benzamide, 2-fluoro-N-propyl-

Inchi:	InChI=1S/C10H12FNO/c1-2-7-12-10(13)8-5-3-4-6-9(8)11/h3-6H,2,7H2,1H3,(H,12,13)
InchiKey:	UJNVPTNAUICCCU-UHFFFAOYSA-N
Formula:	C10H12FNO
SMILES:	CCCN=C(O)c1ccccc1F
Mol. weight [g/mol]:	181.21

Physical Properties

Property code	Value	Unit	Source
hf	-300.58	kJ/mol	Joback Method
hvap	60.05	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.540		Crippen Method
mcvol	141.320	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	1488.00		NIST Webbook
rinpol	1488.00		NIST Webbook
tb	627.87	K	Joback Method
tc	830.63	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=U407129&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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