

Benzamide, N-(4-fluorophenyl)-4-ethyl-

Inchi:	InChI=1S/C15H14FNO/c1-2-11-3-5-12(6-4-11)15(18)17-14-9-7-13(16)8-10-14/h3-10H,2H
InchiKey:	KAXCAIMITMCVPC-UHFFFAOYSA-N
Formula:	C15H14FNO
SMILES:	CCc1ccc(C(O)=Nc2ccc(F)cc2)cc1
Mol. weight [g/mol]:	243.28

Physical Properties

Property code	Value	Unit	Source
hf	-178.72	kJ/mol	Joback Method
hvap	74.12	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	4.024		Crippen Method
mcvol	188.010	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinpol	2153.00		NIST Webbook
rinpol	2153.00		NIST Webbook
tb	773.93	K	Joback Method
tc	998.53	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307013&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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