

Benzamide, 2-fluoro-N-(2-ethylhexyl)-

Inchi:	InChI=1S/C15H22FNO/c1-3-5-8-12(4-2)11-17-15(18)13-9-6-7-10-14(13)16/h6-7,9-10,12
InchiKey:	IRLQASDTWHMTCO-UHFFFAOYSA-N
Formula:	C15H22FNO
SMILES:	CCCCC(CC)CN=C(O)c1ccccc1F
Mol. weight [g/mol]:	251.34

Physical Properties

Property code	Value	Unit	Source
hf	-409.06	kJ/mol	Joback Method
hvap	70.79	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	4.347		Crippen Method
mcvol	211.770	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	1918.00		NIST Webbook
rinpol	1918.00		NIST Webbook
tb	741.83	K	Joback Method
tc	937.44	K	Joback Method

Sources

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=U407136&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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