

Benzamide, 2-fluoro-N-undecyl-

Inchi:	InChI=1S/C18H28FNO/c1-2-3-4-5-6-7-8-9-12-15-20-18(21)16-13-10-11-14-17(16)19/h10
InchiKey:	PPDGDIGDFNZUHH-UHFFFAOYSA-N
Formula:	C18H28FNO
SMILES:	CCCCCCCCCCCN=C(O)c1ccccc1F
Mol. weight [g/mol]:	293.42

Physical Properties

Property code	Value	Unit	Source
hf	-465.70	kJ/mol	Joback Method
hvap	77.86	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.661		Crippen Method
mcpvol	254.040	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
rinpol	2326.00		NIST Webbook
rinpol	2326.00		NIST Webbook
tb	810.91	K	Joback Method
tc	1004.02	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=U407141&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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