Benzamide, 3-fluoro-N-octyl-

Inchi: InChI=1S/C15H22FNO/c1-2-3-4-5-6-7-11-17-15(18)13-9-8-10-14(16)12-13/h8-10,12H,2-
InchiKey: PGKTXYJWROIJGF-UHFFFAOYSA-N
Formula: C15H22FNO
SMILES: CCCCCCCCN=C(O)c1cccc(F)c1
Mol. weight [g/mol]: 251.34

Physical Properties

Property code	Value	Unit	Source
hf	-403.78	kJ/mol	Joback Method
hvap	71.18	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.491		Crippen Method
mcvol	211.770	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	2053.00		NIST Webbook
rinpol	2053.00		NIST Webbook
tb	742.27	K	Joback Method
tc	935.31	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=U407285&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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