Benzamide, 3-chloro-2-fluoro-N-heptyl-

Inchi: InChI=1S/C14H19ClFNO/c1-2-3-4-5-6-10-17-14(18)11-8-7-9-12(15)13(11)16/h7-9H,2-6,1

InchiKey: IUQFNYWUYDZIDH-UHFFFAOYSA-N

Formula: C14H19ClFNO

SMILES: CCCCCCCN=C(O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 271.76

Physical Properties

Property code	Value	Unit	Source
hf	-410.35	kJ/mol	Joback Method
hvap	74.00	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.754		Crippen Method
mcvol	209.920	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	2075.00		NIST Webbook
rinpol	2075.00		NIST Webbook
tb	761.80	K	Joback Method
tc	960.77	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=U407826&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