Benzamide, 2-fluoro-N-butyl-

Inchi: InChI=1S/C11H14FNO/c1-2-3-8-13-11(14)9-6-4-5-7-10(9)12/h4-7H,2-3,8H2,1H3,(H,13,1
InchiKey: IJILQXVYUMVRIH-UHFFFAOYSA-N
Formula: C11H14FNO
SMILES: CCCCN=C(O)c1ccccc1F
Mol. weight [g/mol]: 195.23

Physical Properties

Property code	Value	Unit	Source
hf	-321.22	kJ/mol	Joback Method
hvap	62.27	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.930		Crippen Method
mcvol	155.410	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	1589.00		NIST Webbook
rinpol	1589.00		NIST Webbook
tb	650.75	K	Joback Method
tc	850.80	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=U407131&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

Latest version available from:

https://www.chemeo.com/cid/94-972-9/Benzamide-2-fluoro-N-butyl.pdf

Generated by Cheméo on 2024-10-12 08:26:16.352484623 +0000 UTC m=+3302438.989453876.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.