

Benzamide, 3-fluoro-N-dodecyl-

Inchi: InChI=1S/C19H30FNO/c1-2-3-4-5-6-7-8-9-10-11-15-21-19(22)17-13-12-14-18(20)16-17/
InchiKey: RUTQPSKIAOCCDE-UHFFFAOYSA-N
Formula: C19H30FNO
SMILES: CCCCCCCCCCN=C(O)c1cccc(F)c1
Mol. weight [g/mol]: 307.45

Physical Properties

Property code	Value	Unit	Source
hf	-486.34	kJ/mol	Joback Method
hvap	80.08	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	6.051		Crippen Method
mcvol	268.130	ml/mol	McGowan Method
pc	1294.86	kPa	Joback Method
rinpol	2472.00		NIST Webbook
rinpol	2472.00		NIST Webbook
tb	833.79	K	Joback Method
tc	1028.20	K	Joback Method

Sources

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=U407289&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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