

N'-(3-fluoro-phenyl)-N,N-dimethyl-acetamide

Inchi: InChI=1S/C10H13FN2/c1-8(13(2)3)12-10-6-4-5-9(11)7-10/h4-7H,1-3H3
InchiKey: JOAFEABQTYBGEC-UHFFFAOYSA-N
Formula: C10H13FN2
SMILES: CC(=Nc1cccc(F)c1)N(C)C
Mol. weight [g/mol]: 180.22

Physical Properties

Property code	Value	Unit	Source
hf	-80.82	kJ/mol	Joback Method
hvap	45.41	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.437		Crippen Method
mcvol	145.430	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
rinpol	1467.00		NIST Webbook
tb	548.13	K	Joback Method
tc	762.92	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R153274&Units=SI>
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

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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