2-Fluoro-6-trifluoromethylbenzamide, N-(3-methylphenyl)-

Inchi: InChI=1S/C15H11F4NO/c1-9-4-2-5-10(8-9)20-14(21)13-11(15(17,18)19)6-3-7-12(13)16/h

InchiKey: IONFLQOKCIJWDI-UHFFFAOYSA-N

Formula: C15H11F4NO

SMILES: Cc1cccc(N=C(O)c2c(F)cccc2C(F)(F)F)c1

Mol. weight [g/mol]: 297.25

Physical Properties

Property code	Value	Unit	Source
hf	-787.27	kJ/mol	Joback Method
hvap	71.03	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.789		Crippen Method
mcvol	193.320	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
rinpol	1986.00		NIST Webbook
rinpol	1986.00		NIST Webbook
tb	773.49	K	Joback Method
tc	984.78	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U358114&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