

3-Fluoro-5-trifluoromethylbenzamide, N-(3-methylphenyl)-

Inchi:	InChI=1S/C15H11F4NO/c1-9-3-2-4-13(5-9)20-14(21)10-6-11(15(17,18)19)8-12(16)7-10/
InchiKey:	NNJNZHHBEGWOLG-UHFFFAOYSA-N
Formula:	C15H11F4NO
SMILES:	Cc1cccc(NC(=O)c2cc(F)cc(C(F)(F)F)c2)c1
Mol. weight [g/mol]:	297.25

Physical Properties

Property code	Value	Unit	Source
gf	-544.58	kJ/mol	Joback Method
hf	-766.58	kJ/mol	Joback Method
hfus	33.12	kJ/mol	Joback Method
hvap	64.14	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.405		Crippen Method
mvol	193.320	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	1962.00		NIST Webbook
rinpol	1962.00		NIST Webbook
tb	708.79	K	Joback Method
tc	922.89	K	Joback Method
tf	456.58	K	Joback Method
vc	0.761	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.18	J/molxK	708.79	Joback Method
cpg	536.84	J/molxK	744.47	Joback Method
cpg	548.52	J/molxK	780.16	Joback Method
cpg	559.28	J/molxK	815.84	Joback Method
cpg	569.18	J/molxK	851.52	Joback Method
cpg	578.30	J/molxK	887.21	Joback Method
cpg	586.70	J/molxK	922.89	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=U358144&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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