

5-Amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]pyrazole-3-carbonitrile

Other names:	1H-Pyrazole-3-carbonitrile, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-[(trifluoromethyl)sulfinyl]pyrazole-3-carbonitrile, 5-Amino-3-cyano-1-(2,6-dichloro-4-trifluoromethylphenyl)-4-trifluoromethylsulfinylpyrazole Fipronil
Inchi:	1-(2,6-Dichloro-4-trifluoromethylphenyl)-3-cyano-5-amino-4-(trifluoromethylsulfinyl)pyrazole (Fipronil) <chem>N#Cc1nn(-c2c(Cl)cc(C(F)(F)F)cc2Cl)c(N)c1S(=O)C(F)(F)F</chem>
InchiKey:	ZOCSXAVNDGMNBV-UHFFFAOYSA-N
Formula:	C12H4Cl2F6N4OS
SMILES:	<chem>N#Cc1nn(-c2c(Cl)cc(C(F)(F)F)cc2Cl)c(N)c1S(=O)C(F)(F)F</chem>
Mol. weight [g/mol]:	437.15
CAS:	120068-37-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.00		Crippen Method
logp	4.279		Crippen Method
mcpol	225.360	ml/mol	McGowan Method
rinpol	2069.00		NIST Webbook
rinpol	2059.00		NIST Webbook
rinpol	2052.00		NIST Webbook
rinpol	2049.00		NIST Webbook
rinpol	2069.00		NIST Webbook
rinpol	2052.00		NIST Webbook
rinpol	2052.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	85.00	kJ/mol	398.00	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C120068373&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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