Diflufenican

Other names:	3-Pyridinecarboxamide, N-(2,4-difluorophenyl)-2-[3-(trifluoromethyl)phenoxy]- Diflufenicam N-(2,4-difluorophenyl)-2-(3-(trifluoromethyl)phenoxy)nicotinamide N-(2,4-difluorophenyl)-2-[3-(trifluoro-methyl)phenoxyl]-3-pyridine carboxamide N-(2,4-difluorophenyl)-2-[3-(trifluoromethyl)phenoxy]pyridine-3-carboxamide
Inchi:	InChI=1S/C19H11F5N2O2/c20-12-6-7-16(15(21)10-12)26-17(27)14-5-2-8-25-18(14)28-1
InchiKey:	WYEHFWKAOXOVJD-UHFFFAOYSA-N
Formula:	C19H11F5N2O2
SMILES:	O=C(Nc1ccc(F)cc1F)c1cccnc1Oc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	394.29
CAS:	83164-33-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.90		Aqueous Solubility Prediction Method
logp	5.423		Crippen Method
mcvol	243.540	ml/mol	McGowan Method
rinpol	2396.00		NIST Webbook
rinpol	2397.00		NIST Webbook
rinpol	2397.00		NIST Webbook
tf	435.52	K	Solubility of Diflufenican in Pure and Binary Solvent Systems

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83164334&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of Diflufenican in Pure and Binary Solvent Systems:	https://www.doi.org/10.1021/acs.jced.8b00632

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

Latest version available from:
https://www.chemeo.com/cid/39-693-0/Diflufenican.pdf
Generated by Cheméo on 2024-04-20 04:04:24.706072223 +0000 UTC m=+15875113.626649534.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.