

TRIFLOXYSTROBIN

Other names:	Benzeneacetic acid, «alpha»-(methoxyimino)-2-[[[(E)-[1-[3-(trifluoromethyl)phenyl]ethylidene]amino]oxy]methyl]methyl ester, («alpha»E)-[«alpha»E]-«alpha»-(methoxyimino)-2-[[[(1E)-1-[3-(trifluoromethyl)phenyl]ethylidene]amino]oxy]methyl ester
Inchi:	InChI=1S/C20H19F3N2O4/c1-13(14-8-6-9-16(11-14)20(21,22)23)24-29-12-15-7-4-5-10
InchiKey:	ONCZDRURRATYFI-UHFFFAOYSA-N
Formula:	C20H19F3N2O4
SMILES:	CON=C(C(=O)OC)c1ccccc1CON=C(C)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	408.37
CAS:	141517-21-7

Physical Properties

Property code	Value	Unit	Source
hf	-967.47	kJ/mol	Joback Method
hvap	83.01	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.170		Crippen Method
mcvol	280.990	ml/mol	McGowan Method
pc	1266.45	kPa	Joback Method
rinpol	2344.00		NIST Webbook
rinpol	2339.00		NIST Webbook
rinpol	2336.00		NIST Webbook
tb	989.15	K	Joback Method
tc	1224.73	K	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=C141517217&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
r_{inpol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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