Oxyflourfen

Other names:	Benzene, 2-chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)-
	Ether, 2-chloro-«alpha»,«alpha»,«alpha»-trifluoro-p-tolyl 3-ethoxy-4-nitrophenyl
	2-Chloro-1-(3-ethoxy-4-nitrophenoxy)-4-trifluoromethylbenzene
	2-Chloro-«alpha»,«alpha»,«alpha»-trifluoro-p-tolyl-3-ethoxy-4-nitrophenyl ether
	Goal
	Oxyfluorfene
	RH 2915
	Oxyfluorofen
	Galigan
	Koltar
	Oxygold
	Oxyflurofen
Inchi:	InChI=1S/C15H11ClF3NO4/c1-2-23-14-8-10(4-5-12(14)20(21)22)24-13-6-3-9(7-11(13)16
InchiKey:	OQMBBFQZGJFLBU-UHFFFAOYSA-N
Formula:	C15H11ClF3NO4
SMILES:	CCOc1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]:	361.70

Physical Properties

Property code	Value	Unit	Source
hfus	40.89	kJ/mol	Joback Method
log10ws	-6.50		Cheméo Relay (1.0)
logp	5.458		Crippen Method
mcvol	221.400	ml/mol	McGowan Method
rinpol	2198.00		NIST Webbook
rinpol	2197.00		NIST Webbook
tb	625.60	K	Cheméo Relay (1.0)
tf	359.75 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.53	J/mol×K	844.57	Joback Method
cpg	632.33	J/mol×K	883.82	Joback Method

cpg	642.05	J/mol×K	923.07	Joback Method
cpg	650.74	J/mol×K	962.33	Joback Method
cpg	658.45	J/mol×K	1001.58	Joback Method
cpg	665.23	J/mol×K	1040.83	Joback Method
cpg	671.11	J/mol×K	1080.08	Joback Method
hfust	30.07	kJ/mol	358.80	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42874033&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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