Oxyfluorfen

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
CAS:	42874-03-3

Physical Properties

Property code	Value	Unit	Source
gf	-506.25	kJ/mol	Joback Method
hf	-813.77	kJ/mol	Joback Method
hfus	40.89	kJ/mol	Joback Method
hvap	78.23	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.458		Crippen Method
mcvol	221.400	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpol	2197.00		NIST Webbook
rinpol	2198.00		NIST Webbook
tb	844.57	K	Joback Method
tc	1080.08	K	Joback Method
tf	359.75 ± 0.20	K	NIST Webbook
vc	0.870	m3/kmol	Joback Method

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

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=C42874033&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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
hfust: Enthalpy of fusion at a given temperature
hvap: 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume