Fluorodifen

Other names:	2,4'-Dinitro-4-(trifluoromethyl)diphenyl ether
	2,4-Dinitro-p-trifluoromethyl phenyl ether
	2-Nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)benzene
	4-Nitrophenyl 4-(trifluoromethyl)-2-nitrophenyl ether
	4-Nitrophenyl «alpha»,«alpha»,«alpha»-trifluoro-2-nitro-p-tolyl ether
	4-Trifluoromethyl-2,4'-dinitrodiphenyl ether
	4-Trifluoromethyl-2,4'-dinitrophenyl ether
	Benzene, 2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)-
	C 6989
	Ether, 2,4'-dinitro-4-trifluoromethyldiphenyl
	Ether, p-nitrophenyl «alpha»,«alpha»,«alpha»-trifluoro-2-nitro-p-tolyl
	Fluordifen
	Fluorodiphen
	NSC 58415
	Preforan
	Soyex
	p-Nitrophenyl 2-nitro-4-(trifluoromethyl)phenyl ether
	p-Nitrophenyl «alpha»,«alpha»,«alpha»-trifluoro-2-nitro-p-tolyl ether
Inchi:	InChI=1S/C13H7F3N2O5/c14-13(15,16)8-1-6-12(11(7-8)18(21)22)23-10-4-2-9(3-5-10)17
InchiKey:	HHMCAJWVGYGUEF-UHFFFAOYSA-N
Formula:	C13H7F3N2O5
SMILES:	O=[N+]([O-])c1ccc(Oc2ccc(C(F)(F)F)cc2[N+](=O)[O-])cc1
Mol. weight [g/mol]:	328.20
CAS:	15457-05-3

Physical Properties

Property code	Value	Unit	Source
gf	-360.98	kJ/mol	Joback Method
hf	-623.82	kJ/mol	Joback Method
hfus	42.08	kJ/mol	Joback Method
hvap	82.92	kJ/mol	Joback Method
log10ws	-5.22		Aqueous Solubility Prediction Method
logp	4.314		Crippen Method
mcvol	192.530	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
tb	885.82	K	Joback Method

tc	1146.01	K	Joback Method
tf	364.88 ± 0.20	K	NIST Webbook
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.34	J/mol×K	885.82	Joback Method
cpg	565.19	J/mol×K	929.19	Joback Method
cpg	573.02	J/mol×K	972.55	Joback Method
cpg	579.91	J/mol×K	1015.92	Joback Method
cpg	585.96	J/mol×K	1059.28	Joback Method
cpg	591.28	J/mol×K	1102.65	Joback Method
cpg	595.95	J/mol×K	1146.01	Joback Method
hfust	18.44	kJ/mol	364.60	NIST Webbook
hfust	18.44	kJ/mol	364.60	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
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=C15457053&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume