Benzene, 2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)-

Other names: Benzene, 2-nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)-
Ether, p-nitrophenyl «alpha»,«alpha»,«alpha»-trifluoro-2-nitro-p-tolyl
p-Nitrophenyl 2-nitro-4-(trifluoromethyl)phenyl ether
C 6989
Ether, 2,4'-dinitro-4-trifluoromethyldiphenyl
Fluordifen
Fluorodiphen
Preforan
2,4-Dinitro-p-trifluoromethyl phenyl ether
2,4'-Dinitro-4-(trifluoromethyl)diphenyl ether
4-Nitrophenyl 4-(trifluoromethyl)-2-nitrophenyl ether
4-Trifluoromethyl-2,4'-dinitrodiphenyl ether
4-Trifluoromethyl-2,4'-dinitrophenyl ether
p-Nitrophenyl «alpha»,«alpha»,«alpha»-trifluoro-2-nitro-p-tolyl ether
Soyex
2-Nitro-1-(4-nitrophenoxy)-4-(trifluoromethyl)benzene
4-Nitrophenyl «alpha»,«alpha»,«alpha»-trifluoro-2-nitro-p-tolyl ether
NSC 58415

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

Physical Properties

Property code	Value	Unit	Source
hfus	42.08	kJ/mol	Joback Method
ie	9.28	eV	Cheméo Relay (1.0)
log10ws	-5.42		Cheméo Relay (1.0)
logp	4.314		Crippen Method
mcvol	192.530	ml/mol	McGowan Method
tb	607.80	K	Cheméo Relay (1.0)
tf	361.02	K	Cheméo Relay (1.0)

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

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C15457053
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

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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