Trifluralin

Other names:

2,6-Dinitro-N,N-di-n-propyl-«alpha»,«alpha»,«alpha»-trifluoro-p-toluidine
2,6-Dinitro-N,N-di-n-propyl-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-p-toluidine
2,6-Dinitro-N,N-dipropyl-4-(trifluoromethyl)benzenamine
2,6-Dinitro-N,N-dipropyl-4-(trifluoromethyl)benzeneamine
4-(Di-n-propylamino)-3,5-dinitro-1-(trifluoromethyl)benzene
4-(Trifluoromethyl)-2,6-dinitro-N,N-dipropylaniline
Agreflan
Agriflan 24
Agriphlan 24
Benzenamine, 2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)-
Benzeneamine, 2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)-
Brassix
Crisalin
Digermin
Elancolan
Ipersan
L-36352
Lilly 36,352
N,N-Di-n-propyl-2,6-dinitro-4-trifluoromethylaniline
N,N-Dipropyl-4-trifluoromethyl-2,6-dinitroaniline
NCI C00443
Nitran
Nitran K
Olitref
Sinflouran
Super-Treflan
Synfloran
TRIM
Trefanocide
Treficon
Treflam
Treflan
Tri-4
Trifloran
Trifluraline
Triflurex
Trifurex
Trikepin
Trilin
Tristar

	Zeltoxone
	p-Toluidine, «alpha»,«alpha»,«alpha»-trifluoro-2,6-dinitro-N,N-dipropyl-
	p-Toluidine, Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-2,6-dinitro-N,N-dipropyl-
	«alpha»,«alpha»,«alpha»-Trifluoro-2,6-dinitro-N,N-dipropyl-p-toluidine
	Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-Trifluoro-2,6-dinitro-N,N-dipropyl-p-toluidine
Inchi:	InChI=1S/C13H16F3N3O4/c1-3-5-17(6-4-2)12-10(18(20)21)7-9(13(14,15)16)8-11(12)19(
InchiKey:	ZSDSQXJSNMTJDA-UHFFFAOYSA-N
Formula:	C13H16F3N3O4
SMILES:	CCCN(CCC)c1c([N+](=O)[O-])cc(C(F)(F)F)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	335.28
CAS:	1582-09-8

Physical Properties

Property code	Value	Unit	Source
gf	-257.61	kJ/mol	Joback Method
hf	-660.60	kJ/mol	Joback Method
hfus	49.87	kJ/mol	Joback Method
hvap	80.27	kJ/mol	Joback Method
log10ws	-5.68		Estimated Solubility Method
log10ws	-5.68		Aqueous Solubility Prediction Method
logp	4.148		Crippen Method
mcvol	220.400	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	1671.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1674.00		NIST Webbook

rinpol	1665.00		NIST Webbook
rinpol	1660.00		NIST Webbook
ripol	2169.00		NIST Webbook
tb	849.16	K	Joback Method
tc	1073.60	K	Joback Method
tf	322.19 ± 0.20	K	NIST Webbook
tf	322.90 ± 0.20	K	NIST Webbook
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.72	J/mol×K	849.16	Joback Method
cpg	685.33	J/mol×K	886.57	Joback Method
cpg	696.07	J/mol×K	923.97	Joback Method
cpg	706.01	J/mol×K	961.38	Joback Method
cpg	715.24	J/mol×K	998.78	Joback Method
cpg	723.85	J/mol×K	1036.19	Joback Method
cpg	731.90	J/mol×K	1073.60	Joback Method
hfust	22.32	kJ/mol	321.40	NIST Webbook

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1582098&Units=SI
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

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