Trifluralin

Other names:

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

	4-(Trifluoromethyl)-2,6-dinitro-N,N-dipropylaniline
	Super-Treflan
Inchi:	InChI=1S/C13H16F3N3O4/c1-3-5-17(6-4-2)9-7-10(18(20)21)12(13(14,15)16)11(8-9)19(2
InchiKey:	CTBJBOYGANZNCA-UHFFFAOYSA-N
Formula:	C13H16F3N3O4
SMILES:	CCCN(CCC)c1cc([N+](=O)[O-])c(C(F)(F)F)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	335.28
CAS:	75635-23-3

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	-5.46		Crippen Method
logp	4.148		Crippen Method
mcvol	220.400	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
tb	849.16	K	Joback Method
tc	1073.60	K	Joback Method
tf	624.13	K	Joback Method
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
sfust	73.86	J/mol×K	321.40	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75635233&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume