75635233

Other names:

2,6-Dinitro-N,N-di-n-propyl-«alpha»,«alpha»,«alpha»-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
Trifluralin
Triflurex
Trifurex
Trikepin
Trilin
Tristar
Zeltoxone

	p-Toluidine, «alpha»,«alpha»,«alpha»-trifluoro-2,6-dinitro-N,N-dipropyl-
	«alpha»,«alpha»,«alpha»-Trifluoro-2,6-dinitro-N,N-dipropyl-p-toluidine
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

Physical Properties

Property code	Value	Unit	Source
hfus	49.87	kJ/mol	Joback Method
log10ws	-5.79		Cheméo Relay (1.0)
logp	4.148		Crippen Method
mcvol	220.400	ml/mol	McGowan Method
tf	305.50	K	Cheméo Relay (1.0)

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

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

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?ID=C75635233&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
sfust:	Entropy of fusion at a given temperature
tf:	Normal melting (fusion) point