Dinitramine

Other names: 1,3-Benzenediamine, N1,N1-diethyl-2,6-dinitro-4-(trifluoromethyl)-
1,3-Benzenediamine, N3,N3-diethyl-2,4-dinitro-6-(trifluoromethyl)-
3-Diethylamino-2,4-dinitro-6-trifluoromethylaniline
Cobex
Cobex (herbicide)
Cobexo
N3,N3-Diethyl-2,4-dinitro-6-(trifluoromethyl)-1,3-benzenediamine
N3,N3-Diethyl-2,4-dinitro-6-(trifluoromethyl)-1,3-phenylenediamine
N4,N4-Diethyl-«alpha»,«alpha»,«alpha»-trifluoro-3,5-dinitrotoluene, 2,4-diamine
N4,N4-Diethyl-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-3,5-dinitrotoluene, 2,4-diamine
Nitramine
Toluene-2,4-diamine, N4,N4-diethyl-3,5-dinitro-«alpha»,«alpha»,«alpha»-trifluoro-
Toluene-2,4-diamine, N4,N4-diethyl-3,5-dinitro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-
Toluene-2,4-diamine, N4,N4-diethyl-«alpha»,«alpha»,«alpha»-trifluoro-3,5-dinitro-
Toluene-2,4-diamine, N4,N4-diethyl-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-3,5-dinitro-
USB 3584

Inchi: InChI=1S/C11H13F3N4O4/c1-3-16(4-2)9-7(17(19)20)5-6(11(12,13)14)8(15)10(9)18(21)2

InchiKey: OFDYMSKSGFSLLM-UHFFFAOYSA-N

Formula: C11H13F3N4O4

SMILES: CCN(CC)c1c([N+](=O)[O-])cc(C(F)(F)F)c(N)c1[N+](=O)[O-]

Mol. weight [g/mol]: 322.24

CAS: 29091-05-2

Physical Properties

Property code	Value	Unit	Source
gf	-217.63	kJ/mol	Joback Method
hf	-597.00	kJ/mol	Joback Method
hfus	49.50	kJ/mol	Joback Method
hvap	87.12	kJ/mol	Joback Method
log10ws	-5.47		Aqueous Solubility Prediction Method
log10ws	-3.56		Estimated Solubility Method
logp	2.950		Crippen Method
mcvol	202.200	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
tb	880.91	K	Joback Method

tc	1117.18	K	Joback Method
tf	697.37	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.84	J/mol×K	1077.80	Joback Method
cpg	617.99	J/mol×K	880.91	Joback Method
cpg	627.79	J/mol×K	920.29	Joback Method
cpg	636.80	J/mol×K	959.67	Joback Method
cpg	645.09	J/mol×K	999.04	Joback Method
cpg	652.74	J/mol×K	1038.42	Joback Method
cpg	666.46	J/mol×K	1117.18	Joback Method
hfust	29.13	kJ/mol	372.10	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29091052&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
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

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