Dipicrylamine

Other names:	Hexanitrodiphenylamine
	2,2',4,4',6,6'-Hexanitrodiphenylamine
	Benzenamine, 2,4,6-trinitro-N-(2,4,6-trinitrophenyl)-
	Bis(2,4,6-trinitrophenyl)amine
	Hexyl
	Bis(2,4,6-trinitro-phenyl)-amin
	Diphenylamine, hexanitro-
	Diphenylamine, 2,2',4,4',6,6'-hexanitro-
	Esanitrodifenilamina
	Hexamine
	Hexamine (potassium reagent)
	Hexanitrodifenylamine
	Hexyl (reagent)
	2,4,6-Trinitro-N-(2,4,6-trinitrophenyl)benzenamine
	2,4,6,2',4',6'-Hexanitrodiphenylamine
	Aurantia
	C.I. 10360
	Dipikrylamin
	2,2',4,4',6,6'-Hexanitrodifenylamin
	Hexil
	Hexite
	NSC 1786
Inchi:	InChI=1S/C12H5N7O12/c20-14(21)5-1-7(16(24)25)11(8(2-5)17(26)27)13-12-9(18(28)29)
InchiKey:	CBCIHIVRDWLAME-UHFFFAOYSA-N
Formula:	C12H5N7O12
SMILES:	O=[N+]([O-])c1cc([N+](=O)[O-])c(Nc2c([N+](=O)[O-])cc([N+](=O)[O-])cc2[N+](=O)[O-])c([N
Mol. weight [g/mol]:	439.21
CAS:	131-73-7

Physical Properties

Property code	Value	Unit	Source
chs	-5512.96	kJ/mol	NIST Webbook
chs	-5481.29	kJ/mol	NIST Webbook
gf	519.89	kJ/mol	Joback Method
hf	102.14	kJ/mol	Joback Method
hfs	44.56	kJ/mol	NIST Webbook

hfs	76.27	kJ/mol	NIST Webbook
hfus	85.85	kJ/mol	Joback Method
hvap	156.81	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	2.879		Crippen Method
mcvol	246.920	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
tb	1518.41	K	Joback Method
tc	1863.30	K	Joback Method
tf	1267.28	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.31	J/mol×K	1518.41	Joback Method
cpg	721.45	J/mol×K	1575.89	Joback Method
cpg	719.33	J/mol×K	1633.37	Joback Method
cpg	717.14	J/mol×K	1690.85	Joback Method
cpg	715.05	J/mol×K	1748.33	Joback Method
cpg	713.25	J/mol×K	1805.82	Joback Method
cpg	711.92	J/mol×K	1863.30	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C131737&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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