1,3,6,8-TETRANITROCARBAZOLE

Other names:	9H-Carbazole, 1,3,6,8-tetranitro- Carbazole, 1,3,6,8-tetranitro- Nirosan TNC
Inchi:	InChI=1S/C12H5N5O8/c18-14(19)5-1-7-8-2-6(15(20)21)4-10(17(24)25)12(8)13-11(7)9(3-
InchiKey:	JUSWGNJYSBSOFM-UHFFFAOYSA-N
Formula:	C12H5N5O8
SMILES:	O=[N+]([O-])c1cc([N+](=O)[O-])c2[nH]c3c([N+](=O)[O-])cc([N+](=O)[O-])cc3c2c1
Mol. weight [g/mol]:	347.20

Physical Properties

Property code	Value	Unit	Source
hf	203.67	kJ/mol	Cheméo Relay (1.0)
hvap	130.41	kJ/mol	Cheméo Relay (1.0)
ie	9.24	eV	Cheméo Relay (1.0)
log10ws	-5.41		Cheméo Relay (1.0)
logp	2.472		Crippen Method
mcvol	201.220	ml/mol	McGowan Method
tb	688.33	K	Cheméo Relay (1.0)
tf	579.11	K	Cheméo Relay (1.0)

Sources

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=C4543333&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point