2,2'',4,4',4'',6,6',6''-OCTANITRO-M-TERPHENYL

Other names:	Octanite
	2,2'',4,4',4'',6,6',6''-Octanitro-m-terphenyl
Inchi:	InChI=1S/C18H6N8O16/c27-19(28)7-1-13(23(35)36)17(14(2-7)24(37)38)9-5-10(12(22(33
InchiKey:	ACFBFTOJGUDZAU-UHFFFAOYSA-N
Formula:	C18H6N8O16
SMILES:	O=[N+]([O-])c1cc([N+](=O)[O-])c(-c2cc(-c3c([N+](=O)[O-])cc([N+](=O)[O-])cc3[N+](=O)[O-
Mol. weight [g/mol]:	590.29

Physical Properties

Property code	Value	Unit	Source
chs	-8035.40 ± 8.80	kJ/mol	NIST Webbook
hf	322.09	kJ/mol	Cheméo Relay (1.0)
hfs	95.00 ± 18.00	kJ/mol	NIST Webbook
hfus	111.89	kJ/mol	Joback Method
hvap	160.69	kJ/mol	Cheméo Relay (1.0)
ie	11.16	eV	Cheméo Relay (1.0)
log10ws	-7.17		Cheméo Relay (1.0)
logp	4.286		Crippen Method
mcvol	332.560	ml/mol	McGowan Method
tb	722.76	K	Cheméo Relay (1.0)
tf	511.29	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	949.39	J/mol×K	1950.82	Joback Method
cpg	949.89	J/mol×K	2027.54	Joback Method
cpg	953.07	J/mol×K	2104.27	Joback Method
cpg	959.52	J/mol×K	2180.99	Joback Method
cpg	969.80	J/mol×K	2257.71	Joback Method
cpg	984.50	J/mol×K	2334.44	Joback Method
cpg	1004.19	J/mol×K	2411.16	Joback Method

Sources

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=C33491882&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
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