

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(3
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]:	590.28
CAS:	33491-88-2

Physical Properties

Property code	Value	Unit	Source
chs	-8035.40 ± 8.80	kJ/mol	NIST Webbook
gf	635.64	kJ/mol	Joback Method
hf	105.43	kJ/mol	Joback Method
hfs	95.00 ± 18.00	kJ/mol	NIST Webbook
hfus	111.89	kJ/mol	Joback Method
hvap	201.18	kJ/mol	Joback Method
log10ws	-11.88		Crippen Method
logp	4.286		Crippen Method
mcvol	332.560	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
tb	1950.82	K	Joback Method
tc	2411.16	K	Joback Method
tf	1633.44	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	949.39	J/molxK	1950.82	Joback Method
cpg	949.89	J/molxK	2027.54	Joback Method
cpg	953.07	J/molxK	2104.27	Joback Method
cpg	959.52	J/molxK	2180.99	Joback Method
cpg	969.80	J/molxK	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

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=C33491882&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

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