Benzene, 1,1',1''-methylidynetris[4-nitro-

Other names:	Tris(p-nitrophenyl)methane
	Tris(4-nitrophenyl)methane
	Tri-p-nitrophenylmethane
	Trinitrotriphenylmethane
Inchi:	InChI=1S/C19H13N3O6/c23-20(24)16-7-1-13(2-8-16)19(14-3-9-17(10-4-14)21(25)26)15-
InchiKey:	GFDFIMKBMBRKCK-UHFFFAOYSA-N
Formula:	C19H13N3O6
SMILES:	O=[N+]([O-])c1ccc(C(c2ccc([N+](=O)[O-])cc2)c2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]:	379.32
CAS:	603-49-6

Physical Properties

Property code	Value	Unit	Source
chs	-9509.80	kJ/mol	NIST Webbook
chs	-9509.80	kJ/mol	NIST Webbook
gf	521.65	kJ/mol	Joback Method
hf	202.13	kJ/mol	Joback Method
hfs	175.00	kJ/mol	NIST Webbook
hfs	137.00	kJ/mol	NIST Webbook
hfus	56.48	kJ/mol	Joback Method
hvap	116.09	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	4.591		Crippen Method
mcvol	259.550	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
tb	1184.18	K	Joback Method
tc	1491.29	K	Joback Method
tf	836.54	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.92	J/mol×K	1184.18	Joback Method

cpg	817.49	J/mol×K	1235.36	Joback Method
cpg	824.44	J/mol×K	1286.55	Joback Method
cpg	830.98	J/mol×K	1337.73	Joback Method
cpg	837.34	J/mol×K	1388.92	Joback Method
cpg	843.74	J/mol×K	1440.10	Joback Method
cpg	850.40	J/mol×K	1491.29	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C603496&Units=SI

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