

TRIS(4-NITROPHENYL)METHANE

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]:	379.33

Physical Properties

Property code	Value	Unit	Source
chs	-9509.80	kJ/mol	NIST Webbook
chs	-9509.80	kJ/mol	NIST Webbook
hf	227.72	kJ/mol	Cheméo Relay (1.0)
hfs	137.00	kJ/mol	NIST Webbook
hfs	175.00	kJ/mol	NIST Webbook
hfus	56.48	kJ/mol	Joback Method
hvap	139.64	kJ/mol	Cheméo Relay (1.0)
ie	9.63	eV	Cheméo Relay (1.0)
log10ws	-6.51		Cheméo Relay (1.0)
logp	4.591		Crippen Method
mcvol	259.550	ml/mol	McGowan Method
tb	703.97	K	Cheméo Relay (1.0)
tf	443.91	K	Cheméo Relay (1.0)

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

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=C603496&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

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