

Benzene, 1,2,3,5-tetramethyl-4,6-dinitro-

Other names:	Dinitroisodurene 1,3-Dinitro-2,4,5,6-tetramethylbenzene 4,6-Dinitro-1,2,3,5-tetramethylbenzene Tetramethyl-1,3-dinitrobenzene 1,2,3,5-Tetramethyl-4,6-dinitrobenzene
Inchi:	InChI=1S/C10H12N2O4/c1-5-6(2)9(11(13)14)8(4)10(7(5)3)12(15)16/h1-4H3
InchiKey:	NYUTYKUIBRNYIV-UHFFFAOYSA-N
Formula:	C10H12N2O4
SMILES:	<chem>Cc1c(C)c([N+](=O)[O-])c(C)c([N+](=O)[O-])c1C</chem>
Mol. weight [g/mol]:	224.21
CAS:	4674-22-0

Physical Properties

Property code	Value	Unit	Source
gf	168.68	kJ/mol	Joback Method
hf	-92.07	kJ/mol	Joback Method
hfus	36.47	kJ/mol	Joback Method
hvap	76.62	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	2.737		Crippen Method
mcvol	162.840	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
tb	783.46	K	Joback Method
tc	1040.66	K	Joback Method
tf	480.65 ± 2.00	K	NIST Webbook
vc	0.651	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.82	J/mol×K	783.46	Joback Method
cpg	456.38	J/mol×K	826.33	Joback Method
cpg	467.02	J/mol×K	869.19	Joback Method
cpg	476.75	J/mol×K	912.06	Joback Method

cpg	485.60	J/mol×K	954.93	Joback Method
cpg	493.58	J/mol×K	997.79	Joback Method
cpg	500.73	J/mol×K	1040.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4674220&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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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