4,6-Dinitro-1,3-dimethyl-benzene

Other names:	Benzene, 1,5-dimethyl-2,4-dinitro- m-Xylene, 4,6-dinitro- 4,6-Dinitro-m-xylene 1,3-Dimethyl-4,6-dinitrobenzene 1,5-Dimethyl-2,4-dinitrobenzene 4,6-Dinitro-1,3-xylene
Inchi:	InChI=1S/C8H8N2O4/c1-5-3-6(2)8(10(13)14)4-7(5)9(11)12/h3-4H,1-2H3
InchiKey:	FOWXIRIJHSFCRC-UHFFFAOYSA-N
Formula:	C8H8N2O4
SMILES:	Cc1cc(C)c([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	196.16
CAS:	616-72-8

Physical Properties

Property code	Value	Unit	Source
chs	-4189.40 ± 4.20	kJ/mol	NIST Webbook
gf	171.10	kJ/mol	Joback Method
hf	-27.85	kJ/mol	Joback Method
hfus	32.07	kJ/mol	Joback Method
hvap	70.85	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.120		Crippen Method
mcvol	134.660	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
tb	727.74	K	Joback Method
tc	995.84	K	Joback Method
tf	531.12	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.51	J/mol×K	727.74	Joback Method
cpg	356.93	J/mol×K	772.42	Joback Method

cpg	366.45	J/mol×K	817.11	Joback Method
cpg	375.11	J/mol×K	861.79	Joback Method
cpg	382.95	J/mol×K	906.47	Joback Method
cpg	390.01	J/mol×K	951.16	Joback Method
cpg	396.32	J/mol×K	995.84	Joback Method

Sources

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=C616728&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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