4-METHYL-3,5-DINITROPHENYLAMINE

Other names:	Benzenamine, 4-methyl-3,5-dinitro-
	2,6-Dinitro-4-aminotoluene
	3,5-Dinitro-4-methylaniline
	4-Amino-2,6-dinitrotoluene
	4-ADNT
	4-Methyl-3,5-dinitrobenzenamine
	4-Methyl-3,5-dinitrophenylamine
	3,5-Dinitro-p-toluidine
	NSC 25010
Inchi:	InChI=1S/C7H7N3O4/c1-4-6(9(11)12)2-5(8)3-7(4)10(13)14/h2-3H,8H2,1H3
InchiKey:	KQRJATLINVYHEZ-UHFFFAOYSA-N
Formula:	C7H7N3O4
SMILES:	Cc1c([N+](=O)[O-])cc(N)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	197.15

Physical Properties

Property code	Value	Unit	Source
hf	57.41	kJ/mol	Cheméo Relay (1.0)
hfus	34.68	kJ/mol	Joback Method
hvap	84.22	kJ/mol	Cheméo Relay (1.0)
ie	8.56	eV	Cheméo Relay (1.0)
log10ws	-3.09		Cheméo Relay (1.0)
logp	1.394		Crippen Method
mcvol	130.550	ml/mol	McGowan Method
rinpol	321.91		NIST Webbook
rinpol	321.91		NIST Webbook
tb	584.16	K	Cheméo Relay (1.0)
tf	405.58	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.91	J/mol×K	777.39	Joback Method
cpg	354.86	J/mol×K	823.71	Joback Method

cpg	362.94	J/mol×K	870.02	Joback Method
cpg	370.17	J/mol×K	916.34	Joback Method
cpg	376.61	J/mol×K	962.66	Joback Method
cpg	382.30	J/mol×K	1008.97	Joback Method
cpg	387.28	J/mol×K	1055.29	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19406510&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Legend

cpg: Ideal gas heat capacity
hf: 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point