Benzene, 2-chloro-5-methyl-1,3-dinitro-

Other names: 4-chloro-3,5-dinitrotoluene
Inchi: InChI=1S/C7H5ClN2O4/c1-4-2-5(9(11)12)7(8)6(3-4)10(13)14/h2-3H,1H3
InchiKey: JMDVARRGYWIJGZ-UHFFFAOYSA-N
Formula: C7H5ClN2O4
SMILES: Cc1cc([N+](=O)[O-])c(Cl)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 216.58
CAS: 5264-65-3

Physical Properties

Property code	Value	Unit	Source
gf	150.75	kJ/mol	Joback Method
hf	-22.95	kJ/mol	Joback Method
hfus	33.68	kJ/mol	Joback Method
hvap	73.00	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	2.465		Crippen Method
mcvol	132.810	ml/mol	McGowan Method
pc	3824.55	kPa	Joback Method
tb	742.29	K	Joback Method
tc	1018.71	K	Joback Method
tf	549.77	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.87	J/mol×K	742.29	Joback Method
cpg	324.39	J/mol×K	788.36	Joback Method
cpg	332.09	J/mol×K	834.43	Joback Method
cpg	338.99	J/mol×K	880.50	Joback Method
cpg	345.16	J/mol×K	926.57	Joback Method
cpg	350.62	J/mol×K	972.64	Joback Method
cpg	355.42	J/mol×K	1018.71	Joback Method

Sources

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=C5264653&Units=SI
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
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