2,6-Dichloro-3-nitrotoluene

Other names: Benzene, 1,3-dichloro-2-methyl-4-nitro-
Inchi: InChI=1S/C7H5Cl2NO2/c1-4-5(8)2-3-6(7(4)9)10(11)12/h2-3H,1H3
InchiKey: WBNZUUIFTPNYRN-UHFFFAOYSA-N
Formula: C7H5Cl2NO2
SMILES: Cc1c(Cl)ccc([N+](=O)[O-])c1Cl
Mol. weight [g/mol]: 206.03
CAS: 29682-46-0

Physical Properties

Property code	Value	Unit	Source
gf	103.27	kJ/mol	Joback Method
hf	-27.93	kJ/mol	Joback Method
hfus	26.52	kJ/mol	Joback Method
hvap	60.80	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.210		Crippen Method
mcvol	127.630	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
tb	627.88	K	Joback Method
tc	887.04	K	Joback Method
tf	436.08	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.32	J/mol×K	627.88	Joback Method
cpg	269.10	J/mol×K	671.07	Joback Method
cpg	277.20	J/mol×K	714.27	Joback Method
cpg	284.64	J/mol×K	757.46	Joback Method
cpg	291.45	J/mol×K	800.65	Joback Method
cpg	297.66	J/mol×K	843.84	Joback Method
cpg	303.31	J/mol×K	887.04	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C29682460&Units=SI

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