2-Iodo-4-nitrotoluene

Other names: Benzene, 2-iodo-1-methyl-4-nitro-
Toluene, 2-iodo-4-nitro
Inchi: InChI=1S/C7H6INO2/c1-5-2-3-6(9(10)11)4-7(5)8/h2-4H,1H3
InchiKey: BUQSRXQJUZTIEW-UHFFFAOYSA-N
Formula: C7H6INO2
SMILES: Cc1ccc([N+](=O)[O-])cc1I
Mol. weight [g/mol]: 263.03
CAS: 7745-92-8

Physical Properties

Property code	Value	Unit	Source
gf	194.88	kJ/mol	Joback Method
hf	91.89	kJ/mol	Joback Method
hfus	22.92	kJ/mol	Joback Method
hvap	60.74	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.508		Crippen Method
mcvol	128.970	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
tb	641.18	K	Joback Method
tc	923.86	K	Joback Method
tf	421.78	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.23	J/mol×K	641.18	Joback Method
cpg	266.72	J/mol×K	688.29	Joback Method
cpg	275.37	J/mol×K	735.41	Joback Method
cpg	283.23	J/mol×K	782.52	Joback Method
cpg	290.37	J/mol×K	829.63	Joback Method
cpg	296.86	J/mol×K	876.74	Joback Method
cpg	302.77	J/mol×K	923.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7745928&Units=SI
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

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