

2-Iodo-3-nitrotoluene

Other names:	Toluene, 2-iodo-3-nitro
Inchi:	InChI=1S/C7H6INO2/c1-5-3-2-4-6(7(5)8)9(10)11/h2-4H,1H3
InchiKey:	AKYPSJARSQSCHJ-UHFFFAOYSA-N
Formula:	C7H6INO2
SMILES:	Cc1cccc([N+](=O)[O-])c1I
Mol. weight [g/mol]:	263.03

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=U334513&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

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