

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:	BUQSRXQJUJTIEW-UHFFFAOYSA-N
Formula:	C7H6INO2
SMILES:	Cc1ccc([N+](=O)[O-])cc1I
Mol. weight [g/mol]:	263.03

Physical Properties

Property code	Value	Unit	Source
hf	110.05	kJ/mol	Cheméo Relay (1.0)
hfus	22.92	kJ/mol	Joback Method
hvap	73.65	kJ/mol	Cheméo Relay (1.0)
ie	9.23	eV	Cheméo Relay (1.0)
log10ws	-3.97		Cheméo Relay (1.0)
logp	2.508		Crippen Method
mcvol	128.970	ml/mol	McGowan Method
tb	559.32	K	Cheméo Relay (1.0)
tf	380.12	K	Cheméo Relay (1.0)

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
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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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