3-NITRO-P-TOLUIC ACID

Other names:	p-Toluic acid, 3-nitro-
	3-Nitro-4-methylbenzoic acid
	4-Methyl-3-nitrobenzoic acid
	3-Nitro-p-toluic acid
	3-Nitro-para-toluic acid
Inchi:	InChI=1S/C8H7NO4/c1-5-2-3-6(8(10)11)4-7(5)9(12)13/h2-4H,1H3,(H,10,11)
InchiKey:	BBEWSMNRCUXQRF-UHFFFAOYSA-N
Formula:	C8H7NO4
SMILES:	Cc1ccc(C(=O)O)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	181.15

Physical Properties

Property code	Value	Unit	Source
hf	-310.41	kJ/mol	Cheméo Relay (1.0)
hfus	26.79	kJ/mol	Joback Method
hsub	118.60 ± 2.50	kJ/mol	NIST Webbook
hvap	94.17	kJ/mol	Cheméo Relay (1.0)
ie	9.78	eV	Cheméo Relay (1.0)
log10ws	-2.32		Cheméo Relay (1.0)
logp	1.601		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
tb	554.51	K	Cheméo Relay (1.0)
tc	832.53	K	Cheméo Relay (1.0)
tf	409.62	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.41	J/mol×K	716.97	Joback Method
cpg	322.66	J/mol×K	755.38	Joback Method
cpg	330.28	J/mol×K	793.80	Joback Method
cpg	337.28	J/mol×K	832.21	Joback Method
cpg	343.70	J/mol×K	870.63	Joback Method
cpg	349.56	J/mol×K	909.04	Joback Method

cpg	354.89	J/mol×K	947.46	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C96980&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):

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation 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
tc: Critical Temperature
tf: Normal melting (fusion) point