

2-NITRO-M-TOLUIC ACID

Other names:	3-methyl-2-nitrobenzoic acid
Inchi:	InChI=1S/C8H7NO4/c1-5-3-2-4-6(8(10)11)7(5)9(12)13/h2-4H,1H3,(H,10,11)
InchiKey:	DGDAVTPQCQXLGU-UHFFFAOYSA-N
Formula:	C8H7NO4
SMILES:	Cc1cccc(C(=O)O)c1[N+](=O)[O-]
Mol. weight [g/mol]:	181.15

Physical Properties

Property code	Value	Unit	Source
hf	-304.56	kJ/mol	Cheméo Relay (1.0)
hfus	26.79	kJ/mol	Joback Method
hsub	124.40 ± 2.70	kJ/mol	NIST Webbook
hvap	92.55	kJ/mol	Cheméo Relay (1.0)
ie	9.61	eV	Cheméo Relay (1.0)
log10ws	-2.50		Cheméo Relay (1.0)
logp	1.601		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
tb	551.93	K	Cheméo Relay (1.0)
tc	832.41	K	Cheméo Relay (1.0)
tf	399.21	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):

Study on the Solubilities of
Mononitro-Substituted Products of
NITRO-TOLUIC ACID in Several
Solvents at Temperatures between
297.65 and 351.75 K:

<https://www.doi.org/10.1021/acs.jced.7b00431>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C5437387&Units=SI>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

McGowan Method:

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

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