Benzoic acid, 2-methyl-3-nitro-

Other names:	2-methyl-3-nitrobenzoic acid
	3-Nitro-2-methyl benzoic acid
	3-nitro-o-toluic acid
Inchi:	InChI=1S/C8H7NO4/c1-5-6(8(10)11)3-2-4-7(5)9(12)13/h2-4H,1H3,(H,10,11)
InchiKey:	YPQAFWHSMWWPLX-UHFFFAOYSA-N
Formula:	C8H7NO4
SMILES:	Cc1c(C(=O)O)cccc1[N+](=O)[O-]
Mol. weight [g/mol]:	181.15
CAS:	1975-50-4

Physical Properties

Property code	Value	Unit	Source
gf	-120.56	kJ/mol	Joback Method
hf	-270.43	kJ/mol	Joback Method
hfus	26.79	kJ/mol	Joback Method
hvap	77.02	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	1.601		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	716.97	K	Joback Method
tc	947.46	K	Joback Method
tf	485.74	K	Joback Method
vc	0.482	m3/kmol	Joback Method

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic functions for solubility of 3-nitro-o-toluic acid in nine organic solvents from T = (283.15 to 318.15) K and apparent thermodynamic properties of solutions:	https://www.doi.org/10.1016/j.jct.2017.02.017
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1975504&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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