BENZOIC ACID, 2-METHYL-5-NITRO-

Other names: Benzoic acid, 2-methyl-5-nitro-
5-nitro-o-toluic acid
Inchi: InChI=1S/C8H7NO4/c1-5-2-3-6(9(12)13)4-7(5)8(10)11/h2-4H,1H3,(H,10,11)
InchiKey: DJRFJAVPROZZFL-UHFFFAOYSA-N
Formula: C8H7NO4
SMILES: Cc1ccc([N+](=O)[O-])cc1C(=O)O
Mol. weight [g/mol]: 181.15

Physical Properties

Property code	Value	Unit	Source
hf	-302.04	kJ/mol	Cheméo Relay (1.0)
hfus	26.79	kJ/mol	Joback Method
hvap	93.11	kJ/mol	Cheméo Relay (1.0)
ie	9.66	eV	Cheméo Relay (1.0)
log10ws	-2.25		Cheméo Relay (1.0)
logp	1.601		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
tb	549.16	K	Cheméo Relay (1.0)
tc	834.92	K	Cheméo Relay (1.0)
tf	433.13	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

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1975526&Units=SI

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point