4-METHYL-3-NITROPHENOL

Other names:	2-Nitro-4-hydroxytoluene
	3-Nitro-4-methylphenol
	3-Nitro-p-cresol
	4-Hydroxy-2-nitrotoluene
	Phenol, 4-methyl-3-nitro-
	p-Cresol, 3-nitro-
Inchi:	InChI=1S/C7H7NO3/c1-5-2-3-6(9)4-7(5)8(10)11/h2-4,9H,1H3
InchiKey:	BQEXDUKMTVYBRK-UHFFFAOYSA-N
Formula:	C7H7NO3
SMILES:	Cc1ccc(O)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	153.14
CAS:	2042-14-0

Physical Properties

Property code	Value	Unit	Source
hf	-127.15	kJ/mol	Cheméo Relay (1.0)
hfus	24.68	kJ/mol	Joback Method
hvap	82.00	kJ/mol	Cheméo Relay (1.0)
ie	8.91	eV	Cheméo Relay (1.0)
log10ws	-1.88		Cheméo Relay (1.0)
logp	1.609		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	5008.59	kPa	Joback Method
tb	553.26	K	Cheméo Relay (1.0)
tc	801.77	K	Cheméo Relay (1.0)
tf	350.71	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.28	J/mol×K	623.68	Joback Method
cpg	271.81	J/mol×K	667.01	Joback Method
cpg	280.56	J/mol×K	710.34	Joback Method
cpg	288.66	J/mol×K	753.67	Joback Method

cpg	296.21	J/mol×K	797.01	Joback Method
cpg	303.32	J/mol×K	840.34	Joback Method
cpg	310.10	J/mol×K	883.67	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.01200e+01
Coeff. B	-2.50274e+03
Coeff. C	-8.42820e+01
Temperature range (K), min.	338.82
Temperature range (K), max.	604.76

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):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2042140&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
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point