

5-Methyl-2-nitrophenol

Other names:	2-Nitro-5-methylphenol 3-Hydroxy-4-nitrotoluene 3-Methyl-6-nitrophenol 5-Methyl-2-nitrophenol (3-6) 6-Nitro-m-cresol Phenol, 5-methyl-2-nitro-
Inchi:	InChI=1S/C7H7NO3/c1-5-2-3-6(8(10)11)7(9)4-5/h2-4,9H,1H3
InchiKey:	NQXUSSVLFOBRSE-UHFFFAOYSA-N
Formula:	C7H7NO3
SMILES:	<chem>Cc1ccc([N+](=O)[O-])c(O)c1</chem>
Mol. weight [g/mol]:	153.14
CAS:	700-38-9

Physical Properties

Property code	Value	Unit	Source
gf	-8.23	kJ/mol	Joback Method
hf	-150.82	kJ/mol	Joback Method
hfus	24.68	kJ/mol	Joback Method
hvap	62.80 ± 0.50	kJ/mol	NIST Webbook
log10ws	-2.15		Crippen Method
logp	1.609		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	5008.59	kPa	Joback Method
rinpol	1247.00		NIST Webbook
rinpol	1247.40		NIST Webbook
rinpol	1247.00		NIST Webbook
tb	623.68	K	Joback Method
tc	883.67	K	Joback Method
tf	327.80 ± 0.10	K	NIST Webbook
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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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
hfus	20.79	kJ/mol	302.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.01729e+01
Coeff. B	-2.52676e+03
Coeff. C	-8.42820e+01
Temperature range (K), min.	339.89
Temperature range (K), max.	604.05

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C700389&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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