

Benzene, 2-methyl-1,4-dinitro-

Other names:	1-METHYL-2,5-DINITROBENZENE 2,5-DINITROTOLUENE 2,5-DNT Toluene, 2,5-dinitro-
Inchi:	InChI=1S/C7H6N2O4/c1-5-4-6(8(10)11)2-3-7(5)9(12)13/h2-4H,1H3
InchiKey:	KZBOXYKTSUUBTO-UHFFFAOYSA-N
Formula:	C7H6N2O4
SMILES:	<chem>Cc1cc([N+](=O)[O-])ccc1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	182.13
CAS:	619-15-8

Physical Properties

Property code	Value	Unit	Source
chs	-3578.00	kJ/mol	NIST Webbook
gf	172.31	kJ/mol	Joback Method
hf	4.26	kJ/mol	Joback Method
hfus	29.87	kJ/mol	Joback Method
hvap	67.96	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	1.811		Crippen Method
mcvol	120.570	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
tb	699.88	K	Joback Method
tc	974.05	K	Joback Method
tf	507.33	K	Joback Method
vc	0.483	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.55	J/mol×K	699.88	Joback Method
cpg	309.27	J/mol×K	745.58	Joback Method
cpg	318.09	J/mol×K	791.27	Joback Method
cpg	326.05	J/mol×K	836.97	Joback Method

cpg	333.22	J/mol×K	882.66	Joback Method
cpg	339.64	J/mol×K	928.36	Joback Method
cpg	345.36	J/mol×K	974.05	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.55593e+01
Coeff. B	-5.42545e+03
Coeff. C	-9.77740e+01
Temperature range (K), min.	453.04
Temperature range (K), max.	627.20

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.22766e+02
Coeff. B	-1.51698e+04
Coeff. C	-1.46922e+01
Coeff. D	3.69650e-06
Temperature range (K), min.	325.65
Temperature range (K), max.	814.00

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermopedia.com/research/kdb/hcprop/showprop.php?cmpid=1446
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C619158&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.thermopedia.com/research/kdb/hcprop/showprop.php?cmpid=1446
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

chs:	Standard solid enthalpy of combustion
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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