Phenol, 2,4,6-trinitro-

Other names:	1,3,5-Trinitrophenol
	2,4,6-Trinitrofenol
	2,4,6-Trinitrofenolo
	2,4,6-Trinitrophenyl
	2,4,6-trinitrophenol
	2-Hydroxy-1,3,5-trinitrobenzene
	Acide picrique
	Acido picrico
	C.I. 10305
	Carbazotic Acid
	Hager's reagent
	Kyselina pikrova
	Melinite
	NSC 36947
	Nitroxanthic acid
	Pertite
	Phenol trinitrate
	Picral
	Picronitric acid
	Pikrinezuur
	Pikrinsaeure
	Pikrynowy kwas
	Reflorit
	TNP
	Trinitrophenol
	UN 0154
	picric acid
	picric acid (TNP)
Inchi:	InChI=1S/C6H3N3O7/c10-6-4(8(13)14)1-3(7(11)12)2-5(6)9(15)16/h1-2,10H
InchiKey:	OXNIZHLAWKMVMX-UHFFFAOYSA-N
Formula:	C6H3N3O7
SMILES:	O=[N+]([O-])c1cc([N+](=O)[O-])c(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	229.10
CAS:	88-89-1

Physical Properties

Property code	Value	Unit	Source

hf	-79.15	kJ/mol	Cheméo Relay (1.0)
hfus	44.42	kJ/mol	Joback Method
hvap	87.70	kJ/mol	Cheméo Relay (1.0)
ie	9.94	eV	Cheméo Relay (1.0)
log10ws	-2.83		Aqueous Solubility Prediction Method
logp	1.117		Crippen Method
mcvol	129.770	ml/mol	McGowan Method
tb	531.52	K	Cheméo Relay (1.0)
tf	395.40	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.28	J/mol×K	909.46	Joback Method
cpg	360.02	J/mol×K	959.34	Joback Method
cpg	366.59	J/mol×K	1009.23	Joback Method
cpg	373.16	J/mol×K	1059.11	Joback Method
cpg	379.91	J/mol×K	1108.99	Joback Method
cpg	386.99	J/mol×K	1158.88	Joback Method
cpg	394.59	J/mol×K	1208.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.60634e+01
Coeff. B	-1.28024e+04
Coeff. C	-7.21084e-05
Coeff. D	4.74385e-11
Temperature range (K), min.	468.15
Temperature range (K), max.	598.15

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1469
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solvent Polarity Effect when Amberlite-LA2 Is Used in the Extraction of Picric Acid:	https://www.doi.org/10.1021/acs.jced.6b00970
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubilities and enthalpies of solution of picric acid and picrates at 298.15K in DMF, EtOH and acetic acid:	https://www.doi.org/10.1016/j.tca.2007.04.013
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88891&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point