

Picric acid

Other names:	1,3,5-Trinitrophenol 2,4,6-Trinitrofenol 2,4,6-Trinitrofenolo 2,4,6-Trinitrophenol 2,4,6-Trinitrophenyl 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 Phenol, 2,4,6-trinitro- Picral Picronitric acid Pikrinezuur Pikrinsaeure Pikrynowy kwas Reflorit TNP Trinitrophenol UN 0154 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
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chs	-2571.90 ± 1.70	kJ/mol	NIST Webbook
chs	-2610.00	kJ/mol	NIST Webbook
chs	-2564.88	kJ/mol	NIST Webbook
chs	-2578.60 ± 2.50	kJ/mol	NIST Webbook
chs	-2567.60 ± 2.60	kJ/mol	NIST Webbook
chs	-2569.10 ± 2.60	kJ/mol	NIST Webbook
chs	-2560.00	kJ/mol	NIST Webbook
chs	-2575.90 ± 1.30	kJ/mol	NIST Webbook
gf	44.82	kJ/mol	Joback Method
hf	-163.17	kJ/mol	Joback Method
hfs	-224.90	kJ/mol	NIST Webbook
hfs	-214.00 ± 1.30	kJ/mol	NIST Webbook
hfs	-217.90 ± 2.00	kJ/mol	NIST Webbook
hfus	44.42	kJ/mol	Joback Method
hsub	105.10 ± 1.60	kJ/mol	NIST Webbook
hvap	95.34	kJ/mol	Joback Method
log10ws	-2.83		Aqueous Solubility Prediction Method
logp	1.117		Crippen Method
mcvol	129.770	ml/mol	McGowan Method
pc	5845.00	kPa	Joback Method
tb	909.46	K	Joback Method
tc	1208.76	K	Joback Method
tf	395.00 ± 2.00	K	NIST Webbook
tf	394.10 ± 0.60	K	NIST Webbook
tf	395.60 ± 2.00	K	NIST Webbook
tf	395.15 ± 0.20	K	NIST Webbook
tf	395.40	K	Aqueous Solubility Prediction Method
tf	393.40 ± 0.30	K	NIST Webbook
tf	394.95 ± 0.30	K	NIST Webbook
vc	0.475	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

cpg	360.02	J/mol×K	959.34	Joback Method
cpg	394.59	J/mol×K	1208.76	Joback Method
cps	239.70	J/mol×K	293.00	NIST Webbook
hfust	17.10	kJ/mol	394.10	NIST Webbook
hfust	17.10	kJ/mol	394.10	NIST Webbook
hfust	17.10	kJ/mol	394.10	NIST Webbook
hvapt	106.40	kJ/mol	533.00	NIST Webbook
hvapt	106.40	kJ/mol	533.00	NIST Webbook
sfust	43.40	J/mol×K	394.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88891&Units=SI
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1469
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
Solvent Polarity Effect when Amberlite-LA2 Is Used in the Extraction of Phenol:	https://www.doi.org/10.1021/acs.jced.6b00970
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity

cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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