Picramic acid

Other names:	Phenol, 2-amino-4,6-dinitro-
	2-Amino-4,6-dinitrophenol
	Acide picramique
	C.I. Oxidation Base 21
	Fourrine 4R
	Fourrine 93
	Furro 4R
	Oxidation Base 21
	Zoba 4R
	2,4-Dinitro-6-aminophenol
	4,6-Dinitro-2-aminophenol
	6-Amino-2,4-dinitrophenol
	1-Amino-2-hydroxy-3,5-dinitrobenzene
	NSC 36939
Inchi:	InChI=1S/C6H5N3O5/c7-4-1-3(8(11)12)2-5(6(4)10)9(13)14/h1-2,10H,7H2
InchiKey:	QXYMVUZOGFVPGH-UHFFFAOYSA-N
Formula:	C6H5N3O5
SMILES:	Nc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1O
Mol. weight [g/mol]:	199.12
CAS:	96-91-3

Physical Properties

Property code	Value	Unit	Source
chs	-2829.00	kJ/mol	NIST Webbook
chs	-2832.05	kJ/mol	NIST Webbook
gf	75.72	kJ/mol	Joback Method
hf	-118.62	kJ/mol	Joback Method
hfs	-246.60	kJ/mol	NIST Webbook
hfs	-243.60	kJ/mol	NIST Webbook
hfus	38.26	kJ/mol	Joback Method
hvap	89.39	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	0.791		Crippen Method
mcvol	122.330	ml/mol	McGowan Method
pc	6268.93	kPa	Joback Method
tb	830.15	K	Joback Method
tc	1118.55	K	Joback Method

tf	691.04	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.79	J/mol×K	830.15	Joback Method
cpg	338.03	J/mol×K	878.22	Joback Method
cpg	344.92	J/mol×K	926.28	Joback Method
cpg	351.59	J/mol×K	974.35	Joback Method
cpg	358.20	J/mol×K	1022.41	Joback Method
cpg	364.89	J/mol×K	1070.48	Joback Method
cpg	371.80	J/mol×K	1118.55	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C96913&Units=SI

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
hfs: Solid phase 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

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume