

2,4,6-Trinitrophenyl-hydrazine

Other names:	Hydrazine, (2,4,6-trinitrophenyl)-
Inchi:	InChI=1S/C6H5N5O6/c7-8-6-4(10(14)15)1-3(9(12)13)2-5(6)11(16)17/h1-2,8H,7H2
InchiKey:	HCTZYGGLKQYBKK-UHFFFAOYSA-N
Formula:	C6H5N5O6
SMILES:	<chem>NNc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	243.13
CAS:	653-49-6

Physical Properties

Property code	Value	Unit	Source
chs	-3116.60	kJ/mol	NIST Webbook
chs	-3112.10	kJ/mol	NIST Webbook
gf	345.65	kJ/mol	Joback Method
hf	89.93	kJ/mol	Joback Method
hfs	36.50	kJ/mol	NIST Webbook
hfs	40.90	kJ/mol	NIST Webbook
hfus	48.55	kJ/mol	Joback Method
hvap	100.06	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	0.697		Crippen Method
mcvol	143.860	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
tb	956.52	K	Joback Method
tc	1247.69	K	Joback Method
tf	788.11	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.71	J/molxK	956.52	Joback Method
cpg	413.32	J/molxK	1005.05	Joback Method
cpg	418.08	J/molxK	1053.58	Joback Method
cpg	422.04	J/molxK	1102.11	Joback Method

cpg	425.26	J/mol×K	1150.64	Joback Method
cpg	427.81	J/mol×K	1199.17	Joback Method
cpg	429.76	J/mol×K	1247.69	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C653496&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

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