Benzenamine, 2,4,6-trinitro-

Other names: Aniline, 2,4,6-trinitro-
Picramide
2,4,6-Trinitroaniline
Inchi: InChI=1S/C6H4N4O6/c7-6-4(9(13)14)1-3(8(11)12)2-5(6)10(15)16/h1-2H,7H2
InchiKey: IAHOUQOWMXVMEH-UHFFFAOYSA-N
Formula: C6H4N4O6
SMILES: Nc1c([N+](=O)[O-])cc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 228.12
CAS: 489-98-5

Physical Properties

Property code	Value	Unit	Source
chs	-2860.10	kJ/mol	NIST Webbook
chs	-2816.87	kJ/mol	NIST Webbook
gf	256.26	kJ/mol	Joback Method
hf	36.46	kJ/mol	Joback Method
hfs	-115.90	kJ/mol	NIST Webbook
hfs	-72.80	kJ/mol	NIST Webbook
hfus	43.45	kJ/mol	Joback Method
hsub	125.30 ± 0.80	kJ/mol	NIST Webbook
hvap	93.63	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	0.993		Crippen Method
mcvol	133.880	ml/mol	McGowan Method
pc	4994.44	kPa	Joback Method
rinpol	337.56		NIST Webbook
tb	906.35	K	Joback Method
tc	1204.38	K	Joback Method
tf	735.45	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	365.18	J/mol×K	906.35	Joback Method
cpg	371.25	J/mol×K	956.02	Joback Method
cpg	376.44	J/mol×K	1005.69	Joback Method
cpg	380.82	J/mol×K	1055.37	Joback Method
cpg	384.44	J/mol×K	1105.04	Joback Method
cpg	387.36	J/mol×K	1154.71	Joback Method
cpg	389.64	J/mol×K	1204.38	Joback Method
hsubt	115.90	kJ/mol	349.50	NIST Webbook

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=C489985&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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume