Benzene, 2-iodo-1,3,5-trinitro-

Other names: Picryl iodide
1-Iodo-2,4,6-trinitrobenzene
Inchi: InChI=1S/C6H2IN3O6/c7-6-4(9(13)14)1-3(8(11)12)2-5(6)10(15)16/h1-2H
InchiKey: ZECBCPLUOMIFAA-UHFFFAOYSA-N
Formula: C6H2IN3O6
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c(I)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 339.00
CAS: 4436-27-5

Physical Properties

Property code	Value	Unit	Source
gf	247.93	kJ/mol	Joback Method
hf	79.54	kJ/mol	Joback Method
hfus	42.66	kJ/mol	Joback Method
hvap	92.36	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	2.016		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
pc	4480.21	kPa	Joback Method
tb	926.96	K	Joback Method
tc	1246.98	K	Joback Method
tf	710.25	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.15	J/mol×K	926.96	Joback Method
cpg	347.35	J/mol×K	980.30	Joback Method
cpg	351.85	J/mol×K	1033.63	Joback Method
cpg	355.73	J/mol×K	1086.97	Joback Method
cpg	359.11	J/mol×K	1140.31	Joback Method
cpg	362.07	J/mol×K	1193.64	Joback Method
cpg	364.73	J/mol×K	1246.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4436275&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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