3,5-Dinitroiodobenzene

Other names: Benzene, 1-iodo-3,5-dinitro
Inchi: InChI=1S/C6H3IN2O4/c7-4-1-5(8(10)11)3-6(2-4)9(12)13/h1-3H
InchiKey: AISNAASNOWRWIR-UHFFFAOYSA-N
Formula: C6H3IN2O4
SMILES: O=[N+]([O-])c1cc(I)cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 294.00
CAS: 6276-04-6

Physical Properties

Property code	Value	Unit	Source
gf	222.01	kJ/mol	Joback Method
hf	101.77	kJ/mol	Joback Method
hfus	31.69	kJ/mol	Joback Method
hvap	75.10	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	2.108		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	4498.26	kPa	Joback Method
tb	770.14	K	Joback Method
tc	1078.79	K	Joback Method
tf	554.12	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.35	J/mol×K	770.14	Joback Method
cpg	287.34	J/mol×K	821.58	Joback Method
cpg	293.52	J/mol×K	873.02	Joback Method
cpg	298.98	J/mol×K	924.46	Joback Method
cpg	303.82	J/mol×K	975.91	Joback Method
cpg	308.13	J/mol×K	1027.35	Joback Method
cpg	312.00	J/mol×K	1078.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6276046&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

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