2,6-Diiodo-4-nitroaniline

Other names: 2,6-Diiodo-4-nitroaniliine
Benzenamine, 2,6-diiodo-4-nitro-
Inchi: InChI=1S/C6H4I2N2O2/c7-4-1-3(10(11)12)2-5(8)6(4)9/h1-2H,9H2
InchiKey: YPVYMWQYENWFAT-UHFFFAOYSA-N
Formula: C6H4I2N2O2
SMILES: Nc1c(I)cc([N+](=O)[O-])cc1I
Mol. weight [g/mol]: 389.92
CAS: 5398-27-6

Physical Properties

Property code	Value	Unit	Source
gf	301.40	kJ/mol	Joback Method
hf	211.72	kJ/mol	Joback Method
hfus	29.54	kJ/mol	Joback Method
hvap	79.19	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	2.386		Crippen Method
mcvol	150.680	ml/mol	McGowan Method
pc	4546.92	kPa	Joback Method
tb	788.95	K	Joback Method
tc	1111.70	K	Joback Method
tf	564.35	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.16	J/mol×K	788.95	Joback Method
cpg	286.49	J/mol×K	842.74	Joback Method
cpg	292.19	J/mol×K	896.53	Joback Method
cpg	297.36	J/mol×K	950.32	Joback Method
cpg	302.12	J/mol×K	1004.11	Joback Method
cpg	306.59	J/mol×K	1057.91	Joback Method
cpg	310.88	J/mol×K	1111.70	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=C5398276&Units=SI

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