p,«beta»-Dinitrostyrene

Other names:	Benzene, 1-nitro-4-(2-nitroethenyl)-
	Styrene, p,«beta»-dinitro-
	1-Nitro-2-(p-nitrophenyl)ethylene
	2-Nitro-1-(4-nitrophenyl)ethene
	4-Nitro-«beta»-nitrostyrene
	Ethene,-1-(4-nitrophenyl)-2-nitro-
	1-Nitro-4-(2-nitroethenyl)benzene
Inchi:	InChI=1S/C8H6N2O4/c11-9(12)6-5-7-1-3-8(4-2-7)10(13)14/h1-6H/b6-5+
InchiKey:	HABXLWPUIWFTNM-AATRIKPKSA-N
Formula:	C8H6N2O4
SMILES:	O=[N+]([O-])C=Cc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	194.14
CAS:	3156-41-0

Physical Properties

Property code	Value	Unit	Source
chs	-4027.57	kJ/mol	NIST Webbook
gf	270.58	kJ/mol	Joback Method
hf	112.31	kJ/mol	Joback Method
hfus	33.05	kJ/mol	Joback Method
hvap	69.48	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	1.842		Crippen Method
mcvol	130.360	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	721.94	K	Joback Method
tc	999.91	K	Joback Method
tf	501.00	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.64	J/mol×K	721.94	Joback Method

cpg	335.45	J/mol×K	768.27	Joback Method
cpg	344.32	J/mol×K	814.60	Joback Method
cpg	352.34	J/mol×K	860.93	Joback Method
cpg	359.62	J/mol×K	907.25	Joback Method
cpg	366.26	J/mol×K	953.58	Joback Method
cpg	372.36	J/mol×K	999.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3156410&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

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
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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