1,3-Benzodioxole, 5-nitro-

Other names:	1,2-(Methylenedioxy)-4-nitrobenzene
	3,4-(Methylenedioxy)-1-nitrobenzene
	3,4-Methylenedioxynitrobenzene
	5-Nitro-1,3-benzodioxole
	5-Nitrobenzodioxole
	Benzene, 1,2-(methylenedioxy)-4-nitro-
	Methylenedioxynitrobenzene
Inchi:	InChI=1S/C7H5NO4/c9-8(10)5-1-2-6-7(3-5)12-4-11-6/h1-3H,4H2
InchiKey:	SNWQAKNKGGOVMO-UHFFFAOYSA-N
Formula:	C7H5NO4
SMILES:	O=[N+]([O-])c1ccc2c(c1)OCO2
Mol. weight [g/mol]:	167.12
CAS:	2620-44-2

Physical Properties

Property code	Value	Unit	Source
gf	32.98	kJ/mol	Joback Method
hf	-155.84	kJ/mol	Joback Method
hfus	28.20	kJ/mol	Experimental and Computational Thermochemistry of 1,3-Benzodioxole Derivatives
hsub	97.40 ± 2.20	kJ/mol	NIST Webbook
hvap	60.61	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	1.323		Crippen Method
mcvol	104.030	ml/mol	McGowan Method
pc	4876.56	kPa	Joback Method
tb	613.35	K	Joback Method
tc	876.16	K	Joback Method
tf	439.04	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.75	J/mol×K	613.35	Joback Method
cpg	262.37	J/mol×K	657.15	Joback Method
cpg	271.11	J/mol×K	700.95	Joback Method
cpg	279.05	J/mol×K	744.75	Joback Method
cpg	286.29	J/mol×K	788.55	Joback Method
cpg	292.91	J/mol×K	832.35	Joback Method
cpg	299.02	J/mol×K	876.16	Joback Method
hfust	28.20	kJ/mol	420.20	NIST Webbook

Sources

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=C2620442&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and Computational Thermochemistry of 1,3-Benzodioxole Derivatives:	https://www.doi.org/10.1021/je700035m

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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