1,4-Benzodioxin, 2,3-dihydro-6-nitro-

Other names:	1,4-Benzodioxane, 6-nitro-
	6-Nitro-1,4-benzodioxane
	1,4-Benzodioxan, 6-nitro-
	6-Nitro-1,4-benzodioxan
	6-Nitro-2,3-dihydro-benzo[1,4]dioxine
	2,3-dihydro-6-nitro-1,4-benzodioxin
Inchi:	InChI=1S/C8H7NO4/c10-9(11)6-1-2-7-8(5-6)13-4-3-12-7/h1-2,5H,3-4H2
InchiKey:	MQSGCURTKWHBRX-UHFFFAOYSA-N
Formula:	C8H7NO4
SMILES:	O=[N+]([O-])c1ccc2c(c1)OCCO2
Mol. weight [g/mol]:	181.15
CAS:	16498-20-7

Physical Properties

Property code	Value	Unit	Source
gf	29.30	kJ/mol	Joback Method
hf	-182.64	kJ/mol	Joback Method
hfus	32.02	kJ/mol	Joback Method
hvap	63.01	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	1.366		Crippen Method
mcvol	118.120	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
tb	640.50	K	Joback Method
tc	906.22	K	Joback Method
tf	446.79	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.48	J/mol×K	640.50	Joback Method
cpg	310.90	J/mol×K	684.79	Joback Method
cpg	321.30	J/mol×K	729.07	Joback Method

cpg	330.76	J/mol×K	773.36	Joback Method
cpg	339.36	J/mol×K	817.65	Joback Method
cpg	347.20	J/mol×K	861.93	Joback Method
cpg	354.34	J/mol×K	906.22	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=C16498207&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