6-NITROPIPERONAL

Other names:	3,4-(Methylenedioxy)-6-nitrobenzaldehyde
	4,5-Methylenedioxy-2-nitrobenzaldehyde
	1,3-Benzodioxole-5-carboxaldehyde, 6-nitro-
	Piperonal, 6-nitro-
	1,3-Benzodioxole, 5-formyl-6-nitro-
Inchi:	InChI=1S/C8H5NO5/c10-3-5-1-7-8(14-4-13-7)2-6(5)9(11)12/h1-3H,4H2
InchiKey:	NRZWECORTTWSEF-UHFFFAOYSA-N
Formula:	C8H5NO5
SMILES:	O=Cc1cc2c(cc1[N+](=O)[O-])OCO2
Mol. weight [g/mol]:	195.13

Physical Properties

Property code	Value	Unit	Source
hfus	36.02	kJ/mol	Joback Method
log10ws	-3.22		Cheméo Relay (1.0)
logp	1.136		Crippen Method
mcvol	119.690	ml/mol	McGowan Method
tb	576.83	K	Cheméo Relay (1.0)
tf	386.68	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.05	J/mol×K	689.87	Joback Method
cpg	313.68	J/mol×K	732.79	Joback Method
cpg	321.55	J/mol×K	775.71	Joback Method
cpg	328.75	J/mol×K	818.63	Joback Method
cpg	335.36	J/mol×K	861.55	Joback Method
cpg	341.45	J/mol×K	904.47	Joback Method
cpg	347.10	J/mol×K	947.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C712970&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point