6-Nitropiperonyl alcohol

Other names: (6-nitro-1,3-benzodioxol-5-yl)methanol
1,3-Benzodioxole-5-methanol, 6-nitro-
6-Nitro-3,4-methylenedioxybenzyl alcohol
Inchi: InChI=1S/C8H7NO5/c10-3-5-1-7-8(14-4-13-7)2-6(5)9(11)12/h1-2,10H,3-4H2
InchiKey: XSKQKDTZQNFCCB-UHFFFAOYSA-N
Formula: C8H7NO5
SMILES: O=[N+]([O-])c1cc2c(cc1CO)OCO2
Mol. weight [g/mol]: 197.14
CAS: 15341-08-9

Physical Properties

Property code	Value	Unit	Source
gf	-105.05	kJ/mol	Joback Method
hf	-340.18	kJ/mol	Joback Method
hfus	37.82	kJ/mol	Joback Method
hvap	80.18	kJ/mol	Joback Method
log10ws	-3.06		Aqueous Solubility Prediction Method
logp	0.816		Crippen Method
mcvol	123.990	ml/mol	McGowan Method
pc	4749.69	kPa	Joback Method
tb	733.39	K	Joback Method
tc	967.59	K	Joback Method
tf	523.65	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.90	J/mol×K	733.39	Joback Method
cpg	343.99	J/mol×K	772.42	Joback Method
cpg	351.50	J/mol×K	811.46	Joback Method
cpg	358.47	J/mol×K	850.49	Joback Method
cpg	364.98	J/mol×K	889.53	Joback Method

cpg	371.09	J/mol×K	928.56	Joback Method
cpg	376.86	J/mol×K	967.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15341089&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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