

1,3-Benzodioxole, 5-hydroxymethyl-6-nitro-

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:	XSKQKDTZQNFCB-UHFFFAOYSA-N
Formula:	C8H7NO5
SMILES:	O=[N+][O-]c1cc2c(cc1CO)OCO2
Mol. weight [g/mol]:	197.15

Physical Properties

Property code	Value	Unit	Source
hfus	37.82	kJ/mol	Joback Method
log10ws	-3.06		Aqueous Solubility Prediction Method
logp	0.816		Crippen Method
mcvol	123.990	ml/mol	McGowan Method
tb	593.83	K	Cheméo Relay (1.0)

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C15341089&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

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