2-(hydroxymethyl)-6-(3-nitrophenoxy)oxane-3,4,5-

Inchi: InChI=1S/C12H15NO8/c14-5-8-9(15)10(16)11(17)12(21-8)20-7-3-1-2-6(4-7)13(18)19/h1-
InchiKey: VCCMGHVCRFMITI-UHFFFAOYSA-N
Formula: C12H15NO8
SMILES: O=[N+]([O-])c1cccc(OC2OC(CO)C(O)C(O)C2O)c1
Mol. weight [g/mol]: 301.25

Physical Properties

Property code	Value	Unit	Source
gf	-556.30	kJ/mol	Joback Method
hf	-976.89	kJ/mol	Joback Method
hfus	53.49	kJ/mol	Joback Method
hvap	134.66	kJ/mol	Joback Method
log10ws	-1.27		Aqueous Solubility Prediction Method
logp	-1.227		Crippen Method
mcvol	197.960	ml/mol	McGowan Method
pc	3777.68	kPa	Joback Method
tb	1076.42	K	Joback Method
tc	1318.89	K	Joback Method
tf	690.05	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.82	J/mol×K	1076.42	Joback Method
cpg	705.74	J/mol×K	1116.83	Joback Method
cpg	709.21	J/mol×K	1157.24	Joback Method
cpg	711.23	J/mol×K	1197.66	Joback Method
cpg	711.81	J/mol×K	1238.07	Joback Method
cpg	710.97	J/mol×K	1278.48	Joback Method
cpg	708.71	J/mol×K	1318.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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

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