2-(hydroxymethyl)-6-(phenoxy)oxane-3,4,5-triol

Inchi: InChI=1S/C12H16O6/c13-6-8-9(14)10(15)11(16)12(18-8)17-7-4-2-1-3-5-7/h1-5,8-16H,6H
InchiKey: NEZJDVYDSZTRFS-UHFFFAOYSA-N
Formula: C12H16O6
SMILES: OCC1OC(Oc2ccccc2)C(O)C(O)C1O
Mol. weight [g/mol]: 256.25

Physical Properties

Property code	Value	Unit	Source
gf	-582.22	kJ/mol	Joback Method
hf	-954.66	kJ/mol	Joback Method
hfus	42.51	kJ/mol	Joback Method
hvap	117.41	kJ/mol	Joback Method
log10ws	-1.46		Aqueous Solubility Prediction Method
logp	-1.135		Crippen Method
mcvol	180.540	ml/mol	McGowan Method
pc	3791.65	kPa	Joback Method
tb	919.60	K	Joback Method
tc	1126.66	K	Joback Method
tf	438.65	K	Aqueous Solubility Prediction Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.89	J/mol×K	919.60	Joback Method
cpg	633.91	J/mol×K	954.11	Joback Method
cpg	641.90	J/mol×K	988.62	Joback Method
cpg	648.87	J/mol×K	1023.13	Joback Method
cpg	654.83	J/mol×K	1057.64	Joback Method
cpg	659.78	J/mol×K	1092.15	Joback Method
cpg	663.73	J/mol×K	1126.66	Joback Method
dvisc	0.0001127	Pa×s	533.92	Joback Method

dvisc	0.0000233	Pa×s	598.20	Joback Method
dvisc	0.0000065	Pa×s	662.48	Joback Method
dvisc	0.0000023	Pa×s	726.76	Joback Method
dvisc	0.0000010	Pa×s	791.04	Joback Method
dvisc	0.0000005	Pa×s	855.32	Joback Method
dvisc	0.0000002	Pa×s	919.60	Joback Method

Sources

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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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