[2-[[1,3-dihydroxy-2-(hydroxymethyl)propan-2-yl]a
benzoate

Inchi: InChI=1S/C13H17NO6/c15-7-13(8-16,9-17)14-11(18)6-20-12(19)10-4-2-1-3-5-10/h1-5,15

InchiKey: MSMHOCZOEWMZOH-UHFFFAOYSA-N

Formula: C13H17NO6

SMILES: O=C(COC(=O)c1ccccc1)NC(CO)(CO)CO

Mol. weight [g/mol]: 283.28

Physical Properties

Property code	Value	Unit	Source
gf	-510.08	kJ/mol	Joback Method
hf	-844.47	kJ/mol	Joback Method
hfus	37.80	kJ/mol	Joback Method
hvap	117.89	kJ/mol	Joback Method
log10ws	-1.27		Aqueous Solubility Prediction Method
logp	-1.325		Crippen Method
mcvol	206.870	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
tb	977.16	K	Joback Method
tc	1196.32	K	Joback Method
tf	399.65	K	Aqueous Solubility Prediction Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.40	J/mol×K	977.16	Joback Method
cpg	665.26	J/mol×K	1013.69	Joback Method
cpg	672.47	J/mol×K	1050.21	Joback Method
cpg	679.08	J/mol×K	1086.74	Joback Method
cpg	685.16	J/mol×K	1123.27	Joback Method
cpg	690.77	J/mol×K	1159.79	Joback Method
cpg	695.96	J/mol×K	1196.32	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
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