Ribofuranoside, methyl, 5-benzoate, 2,3,-cyclic carbonate, beta-

Inchi: InChI=1S/C14H14O7/c1-17-13-11-10(20-14(16)21-11)9(19-13)7-18-12(15)8-5-3-2-4-6-8/

InchiKey: QEJNCDMZMCHLCH-UHFFFAOYSA-N

Formula: C14H14O7

SMILES: COC1OC(COC(=O)c2ccccc2)C2OC(=O)OC12

Mol. weight [g/mol]: 294.26

CAS: 5517-62-4

Physical Properties

Property code	Value	Unit	Source
gf	-458.58	kJ/mol	Joback Method
hf	-913.88	kJ/mol	Joback Method
hfus	47.69	kJ/mol	Joback Method
hvap	77.93	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.119		Crippen Method
mcvol	195.130	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
tb	806.46	K	Joback Method
tc	1047.15	K	Joback Method
tf	536.64	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.99	J/mol×K	806.46	Joback Method
cpg	639.90	J/mol×K	846.57	Joback Method
cpg	653.32	J/mol×K	886.69	Joback Method
cpg	665.24	J/mol×K	926.80	Joback Method
cpg	675.66	J/mol×K	966.92	Joback Method
cpg	684.60	J/mol×K	1007.03	Joback Method
cpg	692.05	J/mol×K	1047.15	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5517624&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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