Benzene-1,2,3-tricarboxylic acid, 4-hydroxy, trimethyl ester

Inchi: InChI=1S/C12H12O7/c1-17-10(14)6-4-5-7(13)9(12(16)19-3)8(6)11(15)18-2/h4-5,13H,1-3

InchiKey: RLAQYWQGVIWVHJ-UHFFFAOYSA-N

Formula: C12H12O7

SMILES: COC(=O)c1ccc(O)c(C(=O)OC)c1C(=O)OC

Mol. weight [g/mol]: 268.22

Physical Properties

Property code	Value	Unit	Source
gf	-713.07	kJ/mol	Joback Method
hf	-989.13	kJ/mol	Joback Method
hfus	34.24	kJ/mol	Joback Method
hvap	86.39	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	0.752		Crippen Method
mcvol	184.370	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	1871.00		NIST Webbook
rinpol	1871.00		NIST Webbook
tb	820.09	K	Joback Method
tc	1044.63	K	Joback Method
tf	604.66	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.90	J/mol×K	820.09	Joback Method
cpg	527.02	J/mol×K	857.51	Joback Method
cpg	536.38	J/mol×K	894.94	Joback Method
cpg	545.01	J/mol×K	932.36	Joback Method
cpg	552.92	J/mol×K	969.79	Joback Method
cpg	560.12	J/mol×K	1007.21	Joback Method
cpg	566.64	J/mol×K	1044.63	Joback Method
dvisc	0.0000558	Pa×s	604.66	Joback Method

dvisc	0.0000351	Pa×s	640.57	Joback Method
dvisc	0.0000232	Pa×s	676.47	Joback Method
dvisc	0.0000160	Pa×s	712.38	Joback Method
dvisc	0.0000114	Pa×s	748.28	Joback Method
dvisc	0.0000084	Pa×s	784.19	Joback Method
dvisc	0.0000064	Pa×s	820.09	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=R306755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume