Benzene-1,2,4,5-tetracarboxylic acid, 3-methoxy, tetramethyl ester

Inchi: InChI=1S/C15H16O9/c1-20-11-9(14(18)23-4)7(12(16)21-2)6-8(13(17)22-3)10(11)15(19)2

InchiKey: UPEYHHVWWYXENT-UHFFFAOYSA-N

Formula: C15H16O9

SMILES: COC(=O)c1cc(C(=O)OC)c(C(=O)OC)c(OC)c1C(=O)OC

Mol. weight [g/mol]: 340.28

Physical Properties

Property code	Value	Unit	Source
gf	-891.37	kJ/mol	Joback Method
hf	-1273.70	kJ/mol	Joback Method
hfus	39.43	kJ/mol	Joback Method
hvap	92.94	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	0.842		Crippen Method
mcvol	234.080	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	2185.00		NIST Webbook
tb	916.78	K	Joback Method
tc	1135.29	K	Joback Method
tf	646.18	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.05	J/mol×K	916.78	Joback Method
cpg	723.25	J/mol×K	1098.87	Joback Method
cpg	720.16	J/mol×K	1062.45	Joback Method
cpg	715.43	J/mol×K	1026.03	Joback Method
cpg	709.13	J/mol×K	989.62	Joback Method
cpg	701.31	J/mol×K	953.20	Joback Method
cpg	724.65	J/mol×K	1135.29	Joback Method
dvisc	0.0000451	Pa×s	916.78	Joback Method
dvisc	0.0000538	Pa×s	871.68	Joback Method

dvisc	0.0000656	Pa×s	826.58	Joback Method
dvisc	0.0000817	Pa×s	781.48	Joback Method
dvisc	0.0001045	Pa×s	736.38	Joback Method
dvisc	0.0001381	Pa×s	691.28	Joback Method
dvisc	0.0001897	Pa×s	646.18	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R306780&Units=SI

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