Benzene-1,2,4-tricarboxylic acid, 5-methoxy, trimethyl ester

Inchi: InChI=1S/C13H14O7/c1-17-10-6-8(12(15)19-3)7(11(14)18-2)5-9(10)13(16)20-4/h5-6H,1-

InchiKey: AAUNKVZRYQTUNI-UHFFFAOYSA-N

Formula: C13H14O7

SMILES: COC(=O)c1cc(C(=O)OC)c(C(=O)OC)cc1OC

Mol. weight [g/mol]: 282.25

Physical Properties

Property code	Value	Unit	Source
gf	-664.66	kJ/mol	Joback Method
hf	-976.15	kJ/mol	Joback Method
hfus	31.85	kJ/mol	Joback Method
hvap	78.67	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	1.055		Crippen Method
mcvol	198.460	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	2036.00		NIST Webbook
tb	789.75	K	Joback Method
tc	1002.90	K	Joback Method
tf	538.96	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.05	J/mol×K	789.75	Joback Method
cpg	561.62	J/mol×K	825.28	Joback Method
cpg	572.20	J/mol×K	860.80	Joback Method
cpg	581.76	J/mol×K	896.33	Joback Method
cpg	590.26	J/mol×K	931.85	Joback Method
cpg	597.65	J/mol×K	967.38	Joback Method
cpg	603.89	J/mol×K	1002.90	Joback Method
dvisc	0.0003764	Pa×s	538.96	Joback Method
dvisc	0.0002645	Pa×s	580.76	Joback Method

dvisc	0.0001949	Pa×s	622.56	Joback Method
dvisc	0.0001493	Pa×s	664.36	Joback Method
dvisc	0.0001180	Pa×s	706.15	Joback Method
dvisc	0.0000957	Pa×s	747.95	Joback Method
dvisc	0.0000794	Pa×s	789.75	Joback Method

Sources

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=R306824&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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