

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

Inchi:	InChI=1S/C13H14O7/c1-17-8-6-5-7(11(14)18-2)9(12(15)19-3)10(8)13(16)20-4/h5-6H,1-4
InchiKey:	QNFXPXLBMKAQFA-UHFFFAOYSA-N
Formula:	C13H14O7
SMILES:	<chem>COC(=O)c1ccc(OC)c(C(=O)OC)c1C(=O)OC</chem>
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
rinqol	1986.00		NIST Webbook
tb	789.75	K	Joback Method
tc	1002.90	K	Joback Method
tf	538.96	K	Joback Method
vc	0.746	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001949	Paxs	622.56	Joback Method
dvisc	0.0001493	Paxs	664.36	Joback Method
dvisc	0.0001180	Paxs	706.15	Joback Method
dvisc	0.0000957	Paxs	747.95	Joback Method
dvisc	0.0000794	Paxs	789.75	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=R306760&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

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