1,2,4-Benzenetricarboxylic acid, trimethyl ester

Other names: Methyl trimellitate
Trimellitic acid trimethyl ester
Trimethyl trimellitate
Trimethyl 1,2,4-benzenetricarboxylate
1,2,4-Tris(methoxycarbonyl)benzene
trimethyl benzene-1,2,4-tricarboxylate

Inchi: InChI=1S/C12H12O6/c1-16-10(13)7-4-5-8(11(14)17-2)9(6-7)12(15)18-3/h4-6H,1-3H3

InchiKey: MJHNUUNSCNRGJE-UHFFFAOYSA-N

Formula: C12H12O6

SMILES: COC(=O)c1ccc(C(=O)OC)c(C(=O)OC)c1

Mol. weight [g/mol]: 252.22

CAS: 2459-10-1

Physical Properties

Property code	Value	Unit	Source
gf	-558.45	kJ/mol	Joback Method
hf	-811.82	kJ/mol	Joback Method
hfus	28.46	kJ/mol	Joback Method
hvap	73.37	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.046		Crippen Method
mcvol	178.500	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
rinpol	1800.00		NIST Webbook
tb	739.47	K	Joback Method
tc	956.11	K	Joback Method
tf	492.94	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.46	J/mol×K	739.47	Joback Method
cpg	522.27	J/mol×K	920.00	Joback Method

cpg	514.34	J/mol×K	883.89	Joback Method
cpg	505.47	J/mol×K	847.79	Joback Method
cpg	495.68	J/mol×K	811.68	Joback Method
cpg	485.01	J/mol×K	775.58	Joback Method
cpg	529.23	J/mol×K	956.11	Joback Method
dvisc	0.0001164	Pa×s	739.47	Joback Method
dvisc	0.0001418	Pa×s	698.38	Joback Method
dvisc	0.0001770	Pa×s	657.29	Joback Method
dvisc	0.0002275	Pa×s	616.21	Joback Method
dvisc	0.0003031	Pa×s	575.12	Joback Method
dvisc	0.0004222	Pa×s	534.03	Joback Method
dvisc	0.0006214	Pa×s	492.94	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	467.20	K	1.60	NIST Webbook
tbrp	436.00 ± 2.00	K	0.30	NIST Webbook

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=C2459101&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume