1,3,5-Benzenetricarboxylic acid, trimethyl ester

Other names: Trimesic acid trimethyl ester
Trimethyl trimesate
Trimethyl 1,3,5-benzenetricarboxylate
Trimethyl benzene-1,3,5-tricarboxylate

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

InchiKey: RGCHNYAILFZUPL-UHFFFAOYSA-N

Formula: C12H12O6

SMILES: COC(=O)c1cc(C(=O)OC)cc(C(=O)OC)c1

Mol. weight [g/mol]: 252.22

CAS: 2672-58-4

Physical Properties

Property code	Value	Unit	Source
chs	-5336.00 ± 1.00	kJ/mol	NIST Webbook
gf	-558.45	kJ/mol	Joback Method
hf	-811.82	kJ/mol	Joback Method
hfs	-1101.10 ± 1.20	kJ/mol	NIST Webbook
hfus	28.46	kJ/mol	Joback Method
hsub	118.90 ± 0.40	kJ/mol	NIST Webbook
hsub	117.50 ± 0.80	kJ/mol	NIST Webbook
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	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1892.00		NIST Webbook
rinpol	1872.00		NIST Webbook
rinpol	1872.00		NIST Webbook
rinpol	1879.00		NIST Webbook
tb	739.47	K	Joback Method
tc	956.11	K	Joback Method
tf	419.40 ± 0.10	K	NIST Webbook
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.23	J/mol×K	956.11	Joback Method
cpg	473.46	J/mol×K	739.47	Joback Method
cpg	485.01	J/mol×K	775.58	Joback Method
cpg	495.68	J/mol×K	811.68	Joback Method
cpg	505.47	J/mol×K	847.79	Joback Method
cpg	514.34	J/mol×K	883.89	Joback Method
cpg	522.27	J/mol×K	920.00	Joback Method
dvisc	0.0001164	Pa×s	739.47	Joback Method
dvisc	0.0006214	Pa×s	492.94	Joback Method
dvisc	0.0004222	Pa×s	534.03	Joback Method
dvisc	0.0003031	Pa×s	575.12	Joback Method
dvisc	0.0002275	Pa×s	616.21	Joback Method
dvisc	0.0001770	Pa×s	657.29	Joback Method
dvisc	0.0001418	Pa×s	698.38	Joback Method
hfust	17.60	kJ/mol	419.40	NIST Webbook
hsubt	115.90 ± 0.40	kJ/mol	359.00	NIST Webbook
hvapt	75.40	kJ/mol	478.00	NIST Webbook

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=C2672584&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions

hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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