1,4-Benzenedicarboxylic acid, 2,3,5,6-tetrachloro-, dimethyl ester

Other names: 1,4-Benzenedicarboxylic acid, 2,3,5,6-tetrachloro-, dimethyl ester
Terephthalic acid, tetrachloro-, dimethyl ester
Chlorthal-methyl
Dacthal
Dimethyl tetrachloroterephthalate
Dimethyl 2,3,5,6-tetrachloroterephthalate
DAC 4
DAC-893
Tetrachloroterephthalic acid dimethyl ester
Chlorothal-methyl
Dacthalor
Dimethyl 2,3,5,6-tetrachloro-1,4-benzenedicarboxylate
Fatal
2,3,5,6-Tetrachloroterephthalic acid, dimethyl ester
2,3,5,6-Tetrachlorphthalsaure-dimethylester
2,3,5,6-Tetrachloro-1,4-benzenedicarboxilic acid dimethyl ester
2,3,5,6-Tetrachloro-1,4-benzenedicarboxylic acid dimethyl ester
Chlorthal-dimethyl
Dimethyl ester of tetrachloroterephthalic acid
Terechloroterephthalic acid dimethyl ester
Terephthalic acid, 2,3,5,6-tetrachloro-,dimethyl ester
Vegetable turf and ornamental weeder
Chlorthal dimethyl ester
NSC 155745
TCTP
Tetral

Inchi: InChI=1S/C10H6Cl4O4/c1-17-9(15)3-5(11)7(13)4(10(16)18-2)8(14)6(3)12/h1-2H3

InchiKey: NPOJQCVWMSKXDN-UHFFFAOYSA-N

Formula: C10H6Cl4O4

SMILES: COC(=O)c1c(Cl)c(Cl)c(C(=O)OC)c(Cl)c1Cl

Mol. weight [g/mol]: 331.97

Physical Properties

Property code	Value	Unit	Source
hf	-663.57	kJ/mol	Cheméo Relay (1.0)
hfus	36.11	kJ/mol	Joback Method

hvap	92.01	kJ/mol	Cheméo Relay (1.0)
ie	9.54	eV	Cheméo Relay (1.0)
log10ws	-5.59		Cheméo Relay (1.0)
logp	3.873		Crippen Method
mcvol	191.840	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
tb	600.08	K	Cheméo Relay (1.0)
tf	430.58	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.76	J/mol×K	782.08	Joback Method
cpg	423.59	J/mol×K	821.07	Joback Method
cpg	430.69	J/mol×K	860.05	Joback Method
cpg	437.02	J/mol×K	899.04	Joback Method
cpg	442.55	J/mol×K	938.03	Joback Method
cpg	447.25	J/mol×K	977.02	Joback Method
cpg	451.11	J/mol×K	1016.00	Joback Method
dvisc	0.0004626	Pa×s	555.48	Joback Method
dvisc	0.0003493	Pa×s	593.25	Joback Method
dvisc	0.0002728	Pa×s	631.01	Joback Method
dvisc	0.0002191	Pa×s	668.78	Joback Method
dvisc	0.0001801	Pa×s	706.55	Joback Method
dvisc	0.0001510	Pa×s	744.31	Joback Method
dvisc	0.0001288	Pa×s	782.08	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C1861321

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point