

DCPA

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-Tetrachlorophthalsäure-dimethylester 2,3,5,6-Tetrachloro-1,4-benzenedicarboxylic 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:	<chem>COC(=O)c1c(Cl)c(Cl)c(C(=O)OC)c(Cl)c1Cl</chem>
Mol. weight [g/mol]:	331.96
CAS:	65862-98-8

Physical Properties

Property code	Value	Unit	Source
ea	0.77	eV	NIST Webbook

gf	-417.98		kJ/mol	Joback Method
hf	-623.11		kJ/mol	Joback Method
hfus	36.11		kJ/mol	Joback Method
hvap	79.29		kJ/mol	Joback Method
log10ws	-4.70			Crippen Method
logp	3.873			Crippen Method
mcvol	191.840		ml/mol	McGowan Method
pc	2555.92		kPa	Joback Method
rinpol	1988.00			NIST Webbook
rinpol	1960.00			NIST Webbook
rinpol	1960.00			NIST Webbook
rinpol	1985.00			NIST Webbook
rinpol	1988.00			NIST Webbook
rinpol	1960.00			NIST Webbook
rinpol	1977.00			NIST Webbook
rinpol	1977.00			NIST Webbook
tb	782.08		K	Joback Method
tc	1016.00		K	Joback Method
tf	555.48		K	Joback Method
vc	0.732		m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C65862988&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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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