

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

Other names:	1,4-Benzenedicarboxylic acid, 2,3,5,6-tetrachloro- Terephthalic acid, tetrachloro- Tetrachloroterephthalic acid 2,3,5,6-Tetrachloroterephthalic acid Dacthal diacid TCTP (terephthalic acid, tetrachloro)
Inchi:	InChI=1S/C8H2Cl4O4/c9-3-1(7(13)14)4(10)6(12)2(5(3)11)8(15)16/h(H,13,14)(H,15,16)
InchiKey:	KZCBXHSWMMIEQU-UHFFFAOYSA-N
Formula:	C8H2Cl4O4
SMILES:	O=C(O)c1c(Cl)c(Cl)c(C(=O)O)c(Cl)c1Cl
Mol. weight [g/mol]:	303.91

Physical Properties

Property code	Value	Unit	Source
hf	-687.25	kJ/mol	Cheméo Relay (1.0)
hfus	36.73	kJ/mol	Joback Method
ie	9.91	eV	Cheméo Relay (1.0)
logp	3.697		Crippen Method
mcvol	163.660	ml/mol	McGowan Method
rinpol	1941.00		NIST Webbook
rinpol	1941.00		NIST Webbook
ripol	2820.00		NIST Webbook
ripol	2820.00		NIST Webbook
tb	594.31	K	Cheméo Relay (1.0)
tf	526.78	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.90	J/mol×K	875.84	Joback Method
cpg	339.59	J/mol×K	912.38	Joback Method
cpg	342.87	J/mol×K	948.93	Joback Method
cpg	345.75	J/mol×K	985.47	Joback Method
cpg	348.25	J/mol×K	1022.02	Joback Method

cpg	350.36	J/mol×K	1058.56	Joback Method
cpg	352.10	J/mol×K	1095.11	Joback Method
dvisc	0.0001075	Pa×s	610.12	Joback Method
dvisc	0.0000587	Pa×s	654.41	Joback Method
dvisc	0.0000346	Pa×s	698.69	Joback Method
dvisc	0.0000217	Pa×s	742.98	Joback Method
dvisc	0.0000144	Pa×s	787.27	Joback Method
dvisc	0.0000099	Pa×s	831.55	Joback Method
dvisc	0.0000071	Pa×s	875.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2136790&Units=SI
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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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