

1,2,3,4-benzenetetracarboxylic acid, tetramethyl ester

Other names:	1,2,3,4-Tetracarbomethoxybenzene
Inchi:	InChI=1S/C14H14O8/c1-19-11(15)7-5-6-8(12(16)20-2)10(14(18)22-4)9(7)13(17)21-3/h5-
InchiKey:	QDJPGDCRLZYJGQ-UHFFFAOYSA-N
Formula:	C14H14O8
SMILES:	COC(=O)c1ccc(C(=O)OC)c(C(=O)OC)c1C(=O)OC
Mol. weight [g/mol]:	310.26

Physical Properties

Property code	Value	Unit	Source
af	0.9134		Cheméo Relay (1.0)
hf	-1285.61	kJ/mol	Cheméo Relay (1.0)
hfus	36.04	kJ/mol	Joback Method
hvap	80.89	kJ/mol	Cheméo Relay (1.0)
ie	9.74	eV	Cheméo Relay (1.0)
log10ws	-3.01		Cheméo Relay (1.0)
logp	0.833		Crippen Method
mcvol	214.120	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	2058.00		NIST Webbook
tb	607.17	K	Cheméo Relay (1.0)
tc	840.64	K	Cheméo Relay (1.0)
tf	404.70 ± 0.10	K	NIST Webbook
vc	0.798	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.37	J/mol×K	866.50	Joback Method
cpg	654.42	J/mol×K	1084.43	Joback Method
cpg	650.85	J/mol×K	1048.11	Joback Method
cpg	645.92	J/mol×K	1011.79	Joback Method
cpg	639.66	J/mol×K	975.46	Joback Method
cpg	632.12	J/mol×K	939.14	Joback Method
cpg	623.34	J/mol×K	902.82	Joback Method

dvisc	0.0001265	Pa×s	733.33	Joback Method
dvisc	0.0000677	Pa×s	866.50	Joback Method
dvisc	0.0000816	Pa×s	822.11	Joback Method
dvisc	0.0001003	Pa×s	777.72	Joback Method
dvisc	0.0003119	Pa×s	600.16	Joback Method
dvisc	0.0001644	Pa×s	688.94	Joback Method
dvisc	0.0002215	Pa×s	644.55	Joback Method
hfust	40.40	kJ/mol	404.70	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3451023&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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
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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