Tetramethyl pyromellitate

Other names:	Pyromellitic acid tetramethyl ester
	Tetramethyl pyromellitate
	Tetramethyl 1,2,4,5-benzenetetracarboxylate
	Tetramethyl benzene-1,2,4,5-tetracarboxylate
Inchi:	InChI=1S/C14H14O8/c1-19-11(15)7-5-9(13(17)21-3)10(14(18)22-4)6-8(7)12(16)20-2/h5-
InchiKey:	QVEIFJBUBJUUMB-UHFFFAOYSA-N
Formula:	C14H14O8
SMILES:	COC(=O)c1cc(C(=O)OC)c(C(=O)OC)cc1C(=O)OC
Mol. weight [g/mol]:	310.26

Physical Properties

Property code	Value	Unit	Source
af	0.9192		Cheméo Relay (1.0)
chs	-6069.10 ± 2.40	kJ/mol	NIST Webbook
chs	-6077.60 ± 0.91	kJ/mol	NIST Webbook
hf	-1353.20	kJ/mol	NIST Webbook
hf	-1352.00 ± 16.00	kJ/mol	NIST Webbook
hf	-1361.30	kJ/mol	NIST Webbook
hfs	-1432.20 ± 1.20	kJ/mol	NIST Webbook
hfs	-1431.00 ± 2.40	kJ/mol	NIST Webbook
hfs	-1440.30 ± 2.40	kJ/mol	NIST Webbook
hfus	36.04	kJ/mol	Joback Method
hsub	79.00	kJ/mol	NIST Webbook
hsub	143.30 ± 0.80	kJ/mol	NIST Webbook
hsub	135.90 ± 1.30	kJ/mol	NIST Webbook
hvap	77.28	kJ/mol	Cheméo Relay (1.0)
ie	9.88	eV	Cheméo Relay (1.0)
log10ws	-3.02		Cheméo Relay (1.0)
logp	0.833		Crippen Method
mcvol	214.120	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	2095.00		NIST Webbook
rinpol	2095.00		NIST Webbook
tb	611.22	K	Cheméo Relay (1.0)
tc	835.23	K	Cheméo Relay (1.0)
tf	418.00 ± 0.10	K	NIST Webbook
vc	0.803	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	623.34	J/mol×K	902.82	Joback Method
cpg	632.12	J/mol×K	939.14	Joback Method
cpg	639.66	J/mol×K	975.46	Joback Method
cpg	645.92	J/mol×K	1011.79	Joback Method
cpg	650.85	J/mol×K	1048.11	Joback Method
cpg	654.42	J/mol×K	1084.43	Joback Method
dvisc	0.0002215	Pa×s	644.55	Joback Method
dvisc	0.0003119	Pa×s	600.16	Joback Method
dvisc	0.0001644	Pa×s	688.94	Joback Method
dvisc	0.0001265	Pa×s	733.33	Joback Method
dvisc	0.0001003	Pa×s	777.72	Joback Method
dvisc	0.0000816	Pa×s	822.11	Joback Method
dvisc	0.0000677	Pa×s	866.50	Joback Method
hfust	35.70	kJ/mol	416.70	NIST Webbook
hsubt	140.40 ± 0.80	kJ/mol	381.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C635109&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):

Legend

af: Acentric Factor

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc:	Dynamic viscosity
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
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