

1,2,3,5-Benzenetetracarboxylic acid, tetramethyl ester

Other names:	1,2,3,5-Tetracarbomethoxybenzene
Inchi:	InChI=1S/C14H14O8/c1-19-11(15)7-5-8(12(16)20-2)10(14(18)22-4)9(6-7)13(17)21-3/h5-
InchiKey:	RVSRYSJPKQMMZ-UHFFFAOYSA-N
Formula:	C14H14O8
SMILES:	<chem>COC(=O)c1cc(C(=O)OC)c(C(=O)OC)c(C(=O)OC)c1</chem>
Mol. weight [g/mol]:	310.26
CAS:	3034-97-7

Physical Properties

Property code	Value	Unit	Source
gf	-785.16	kJ/mol	Joback Method
hf	-1109.37	kJ/mol	Joback Method
hfus	36.04	kJ/mol	Joback Method
hvap	87.64	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	0.833		Crippen Method
mcvol	214.120	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	2131.00		NIST Webbook
tb	866.50	K	Joback Method
tc	1084.43	K	Joback Method
tf	389.20 ± 0.10	K	NIST Webbook
vc	0.807	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	613.37	J/mol×K	866.50	Joback Method

dvisc	0.0003119	Paxs	600.16	Joback Method
dvisc	0.0000677	Paxs	866.50	Joback Method
dvisc	0.0000816	Paxs	822.11	Joback Method
dvisc	0.0001003	Paxs	777.72	Joback Method
dvisc	0.0001265	Paxs	733.33	Joback Method
dvisc	0.0001644	Paxs	688.94	Joback Method
dvisc	0.0002215	Paxs	644.55	Joback Method
hfust	32.60	kJ/mol	389.20	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.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=C3034977&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
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
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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