Benzenehexacarboxylic acid

Other names:	Mellitic acid
	Hexacarboxybenzene
	Mellic acid
	1,2,3,4,5,6-Benzenehexacarboxylic acid
Inchi:	InChI=1S/C12H6O12/c13-7(14)1-2(8(15)16)4(10(19)20)6(12(23)24)5(11(21)22)3(1)9(17)
InchiKey:	YDSWCNNOKPMOTP-UHFFFAOYSA-N
Formula:	C12H6O12
SMILES:	O=C(O)c1c(C(=O)O)c(C(=O)O)c(C(=O)O)c(C(=O)O)c1C(=O)O
Mol. weight [g/mol]:	342.17
CAS:	517-60-2

Physical Properties

Property code	Value	Unit	Source
gf	-1480.02	kJ/mol	Joback Method
hf	-1700.69	kJ/mol	Joback Method
hfus	53.05	kJ/mol	Joback Method
hvap	188.44	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	-0.124		Crippen Method
mcvol	200.820	ml/mol	McGowan Method
pc	7133.40	kPa	Joback Method
tb	1401.84	K	Joback Method
tc	1892.63	K	Joback Method
tf	978.52	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.45	J/mol×K	1401.84	Joback Method
cpg	548.87	J/mol×K	1483.64	Joback Method
cpg	537.22	J/mol×K	1565.44	Joback Method
cpg	522.62	J/mol×K	1647.23	Joback Method
cpg	505.19	J/mol×K	1729.03	Joback Method

cpg	485.04	J/mol×K	1810.83	Joback Method
cpg	462.31	J/mol×K	1892.63	Joback Method
dvisc	5.3890243e-09	Pa×s	978.52	Joback Method
dvisc	2.2035013e-09	Pa×s	1049.07	Joback Method
dvisc	1.0084774e-09	Pa×s	1119.63	Joback Method
dvisc	5.0636486e-10	Pa×s	1190.18	Joback Method
dvisc	2.7463064e-10	Pa×s	1260.73	Joback Method
dvisc	1.5892720e-10	Pa×s	1331.29	Joback Method
dvisc	9.7175974e-11	Pa×s	1401.84	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C517602&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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