Benzenepentacarboxylic acid

Other names: Pentacarboxy benzene
Inchi: InChI=1S/C11H6O10/c12-7(13)2-1-3(8(14)15)5(10(18)19)6(11(20)21)4(2)9(16)17/h1H,(H
InchiKey: QNSOHXTZPUMONC-UHFFFAOYSA-N
Formula: C11H6O10
SMILES: O=C(O)c1cc(C(=O)O)c(C(=O)O)c(C(=O)O)c1C(=O)O
Mol. weight [g/mol]: 298.16
CAS: 1585-40-6

Physical Properties

Property code	Value	Unit	Source
chs	-3256.40 ± 1.20	kJ/mol	NIST Webbook
gf	-1213.07	kJ/mol	Joback Method
hf	-1403.77	kJ/mol	Joback Method
hfs	-1929.70 ± 1.20	kJ/mol	NIST Webbook
hfus	45.17	kJ/mol	Joback Method
hvap	162.13	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	0.178		Crippen Method
mcvol	179.290	ml/mol	McGowan Method
pc	6631.37	kPa	Joback Method
tb	1227.93	K	Joback Method
tc	1550.54	K	Joback Method
tf	843.98	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.15	J/mol×K	1227.93	Joback Method
cpg	509.21	J/mol×K	1281.70	Joback Method
cpg	508.08	J/mol×K	1335.47	Joback Method
cpg	505.80	J/mol×K	1389.24	Joback Method
cpg	502.42	J/mol×K	1443.00	Joback Method
cpg	497.99	J/mol×K	1496.77	Joback Method

cpg	492.55	J/mol×K	1550.54	Joback Method
dvisc	0.0000002	Pa×s	843.98	Joback Method
dvisc	6.4112602e-08	Pa×s	907.97	Joback Method
dvisc	2.8869119e-08	Pa×s	971.96	Joback Method
dvisc	1.4346038e-08	Pa×s	1035.95	Joback Method
dvisc	7.7333442e-09	Pa×s	1099.95	Joback Method
dvisc	4.4618126e-09	Pa×s	1163.94	Joback Method
dvisc	2.7261549e-09	Pa×s	1227.93	Joback Method

Sources

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=C1585406&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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