1,2,3-Benzenetricarboxylic acid

Other names: Benzene-1,2,3-tricarboxylic acid
Hemimellitic acid
1,2,3-Tricarboxybenzene
Inchi: InChI=1S/C9H6O6/c10-7(11)4-2-1-3-5(8(12)13)6(4)9(14)15/h1-3H,(H,10,11)(H,12,13)(H,
InchiKey: UJMDYLWCYJJYMO-UHFFFAOYSA-N
Formula: C9H6O6
SMILES: O=C(O)c1cccc(C(=O)O)c1C(=O)O
Mol. weight [g/mol]: 210.14
CAS: 569-51-7

Physical Properties

Property code	Value	Unit	Source
chs	-3238.70 ± 0.84	kJ/mol	NIST Webbook
gf	-679.17	kJ/mol	Joback Method
hf	-809.93	kJ/mol	Joback Method
hfs	-1160.40 ± 0.84	kJ/mol	NIST Webbook
hfus	29.39	kJ/mol	Joback Method
hvap	109.50	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	0.781		Crippen Method
mcvol	136.230	ml/mol	McGowan Method
pc	5774.15	kPa	Joback Method
tb	880.11	K	Joback Method
tc	1085.73	K	Joback Method
tf	372.00 ± 3.00	K	NIST Webbook
tf	482.00 ± 2.00	K	NIST Webbook
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.92	J/mol×K	880.11	Joback Method
cpg	371.82	J/mol×K	914.38	Joback Method
cpg	376.27	J/mol×K	948.65	Joback Method

cpg	380.27	J/mol×K	982.92	Joback Method
cpg	383.85	J/mol×K	1017.19	Joback Method
cpg	387.03	J/mol×K	1051.46	Joback Method
cpg	389.82	J/mol×K	1085.73	Joback Method
dvisc	0.0000920	Pa×s	574.90	Joback Method
dvisc	0.0000343	Pa×s	625.77	Joback Method
dvisc	0.0000148	Pa×s	676.64	Joback Method
dvisc	0.0000072	Pa×s	727.50	Joback Method
dvisc	0.0000038	Pa×s	778.37	Joback Method
dvisc	0.0000022	Pa×s	829.24	Joback Method
dvisc	0.0000014	Pa×s	880.11	Joback Method

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=C569517&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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