1,3,5-Benzenetricarboxylic acid

Other names: 1,3,5-tricarboxybenzene
5-carboxyisophthalic acid
Trimesinic acid
benzene-1,3,5-tricarboxylic acid
trimesic acid
trimesitinic acid

Inchi: InChI=1S/C9H6O6/c10-7(11)4-1-5(8(12)13)3-6(2-4)9(14)15/h1-3H,(H,10,11)(H,12,13)(H,

InchiKey: QMKYBPDZANOJGF-UHFFFAOYSA-N

Formula: C9H6O6

SMILES: O=C(O)c1cc(C(=O)O)cc(C(=O)O)c1

Mol. weight [g/mol]: 210.14

CAS: 554-95-0

Physical Properties

Property code	Value	Unit	Source
chs	-3209.00 ± 0.88	kJ/mol	NIST Webbook
gf	-679.17	kJ/mol	Joback Method
hf	-809.93	kJ/mol	Joback Method
hfs	-1190.10 ± 0.88	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	574.90	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.82	J/mol×K	1085.73	Joback Method

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
dvisc	0.0000014	Pa×s	880.11	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
hsubt	159.40	kJ/mol	573.00	NIST Webbook

Sources

Solubility of 1,3,5-Benzenetricarboxylic Acid in Different Solvents:	https://www.doi.org/10.1021/acs.jced.5b00870
Solubilities of 1,3,5-Benzenetricarboxylic Acid and 1,3-Benzenedicarboxylic Acid in Acetic Acid + Water Solvent Mixtures:	https://www.doi.org/10.1021/je800353s
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=C554950&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The solubilities of benzene polycarboxylic acids in water:	https://www.doi.org/10.1016/j.jct.2005.07.007

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