2,4,6-Trihydroxybenzoic acid

Other names:	Phloroglucinol carboxylic acid
	2,4,6-Trichydroxybenzoic acid
	Benzoic acid, 2,4,6-trihydroxy-
	Phloroglucincarboxylic acid
	Phloroglucinic acid
	2,4,6-Trihydroxybenzene carboxylic acid
Inchi:	InChI=1S/C7H6O5/c8-3-1-4(9)6(7(11)12)5(10)2-3/h1-2,8-10H,(H,11,12)
InchiKey:	IBHWREHFNDMRPR-UHFFFAOYSA-N
Formula:	C7H6O5
SMILES:	O=C(O)c1c(O)cc(O)cc1O
Mol. weight [g/mol]:	170.12
CAS:	83-30-7

Physical Properties

Property code	Value	Unit	Source
gf	-609.13	kJ/mol	Joback Method
hf	-748.02	kJ/mol	Joback Method
hfus	30.96	kJ/mol	Joback Method
hvap	95.92	kJ/mol	Joback Method
log10ws	-0.18		Crippen Method
logp	0.502		Crippen Method
mcvol	110.780	ml/mol	McGowan Method
pc	10918.83	kPa	Joback Method
rinpol	1728.00		NIST Webbook
rinpol	1728.00		NIST Webbook
tb	774.15	K	Joback Method
tc	1010.28	K	Joback Method
tf	640.98	K	Joback Method
vc	0.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.19	J/mol×K	774.15	Joback Method

cpg	304.89	J/mol×K	813.51	Joback Method
cpg	310.73	J/mol×K	852.86	Joback Method
cpg	316.89	J/mol×K	892.22	Joback Method
cpg	323.55	J/mol×K	931.57	Joback Method
cpg	330.91	J/mol×K	970.93	Joback Method
cpg	339.13	J/mol×K	1010.28	Joback Method
dvisc	0.0000004	Pa×s	640.98	Joback Method
dvisc	0.0000002	Pa×s	663.17	Joback Method
dvisc	0.0000001	Pa×s	685.37	Joback Method
dvisc	8.1649065e-08	Pa×s	707.57	Joback Method
dvisc	5.1976473e-08	Pa×s	729.76	Joback Method
dvisc	3.3981406e-08	Pa×s	751.95	Joback Method
dvisc	2.2764543e-08	Pa×s	774.15	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C83307&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume