

2,3-Dihydroxybenzaldehyde

Other names:	Benzaldehyde, 2,3-dihydroxy- o-Pyrocatechualdehyde 5,6-Dihydroxybenzaldehyde
Inchi:	InChI=1S/C7H6O3/c8-4-5-2-1-3-6(9)7(5)10/h1-4,9-10H
InchiKey:	IXWOUPGDGMCKGT-UHFFFAOYSA-N
Formula:	C7H6O3
SMILES:	O=Cc1cccc(O)c1O
Mol. weight [g/mol]:	138.12
CAS:	24677-78-9

Physical Properties

Property code	Value	Unit	Source
gf	-288.29	kJ/mol	Joback Method
hf	-391.48	kJ/mol	Joback Method
hfus	21.78	kJ/mol	Joback Method
hvap	66.20	kJ/mol	Joback Method
log10ws	-0.81		Crippen Method
logp	0.910		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	7097.39	kPa	Joback Method
ripol	2318.00		NIST Webbook
tb	596.14	K	Joback Method
tc	841.41	K	Joback Method
tf	460.51	K	Joback Method
vc	0.269	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.91	J/molxK	596.14	Joback Method
cpg	243.43	J/molxK	637.02	Joback Method
cpg	250.27	J/molxK	677.90	Joback Method
cpg	256.59	J/molxK	718.78	Joback Method
cpg	262.52	J/molxK	759.65	Joback Method

cpg	268.22	J/molxK	800.53	Joback Method
cpg	273.83	J/molxK	841.41	Joback Method
dvisc	0.0002085	Paxs	460.51	Joback Method
dvisc	0.0001108	Paxs	483.12	Joback Method
dvisc	0.0000623	Paxs	505.72	Joback Method
dvisc	0.0000368	Paxs	528.33	Joback Method
dvisc	0.0000227	Paxs	550.93	Joback Method
dvisc	0.0000146	Paxs	573.53	Joback Method
dvisc	0.0000096	Paxs	596.14	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.70	K	2.10	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C24677789&Units=SI

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

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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