

2,4,6-Trihydroxybenzaldehyde

Other names:	Phloroglucinol aldehyde Phloroglucinaldehyde Benzaldehyde, 2,4,6-trihydroxy- Formylphloroglucinol
Inchi:	InChI=1S/C7H6O4/c8-3-5-6(10)1-4(9)2-7(5)11/h1-3,9-11H
InchiKey:	BTQAJGSMXCDDAJ-UHFFFAOYSA-N
Formula:	C7H6O4
SMILES:	O=Cc1c(O)cc(O)cc1O
Mol. weight [g/mol]:	154.12
CAS:	487-70-7

Physical Properties

Property code	Value	Unit	Source
gf	-442.91	kJ/mol	Joback Method
hf	-568.79	kJ/mol	Joback Method
hfus	27.57	kJ/mol	Joback Method
hvap	79.21	kJ/mol	Joback Method
log10ws	-0.36		Crippen Method
logp	0.616		Crippen Method
mcvol	104.910	ml/mol	McGowan Method
pc	9281.22	kPa	Joback Method
tb	676.76	K	Joback Method
tc	930.38	K	Joback Method
tf	572.23	K	Joback Method
vc	0.234	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.64	J/molxK	676.76	Joback Method
cpg	299.74	J/molxK	888.11	Joback Method
cpg	293.42	J/molxK	845.84	Joback Method
cpg	287.47	J/molxK	803.57	Joback Method
cpg	281.67	J/molxK	761.30	Joback Method

cpg	275.80	J/molxK	719.03	Joback Method
cpg	306.67	J/molxK	930.38	Joback Method
dvisc	0.0000004	Paxs	676.76	Joback Method
dvisc	0.0000006	Paxs	659.34	Joback Method
dvisc	0.0000009	Paxs	641.92	Joback Method
dvisc	0.0000013	Paxs	624.50	Joback Method
dvisc	0.0000019	Paxs	607.07	Joback Method
dvisc	0.0000029	Paxs	589.65	Joback Method
dvisc	0.0000045	Paxs	572.23	Joback Method

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=C487707&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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