Ethanone, 1-(2,3,4-trihydroxyphenyl)-

Other names:	Gallacetophenone
	Acetophenone, 2',3',4'-trihydroxy-
	Alizarin Yellow C
	Alizarine Yellow C
	C.I. 57000
	Galloacetophenone
	2,3,4-Trihydroxyacetophenone
	2',3',4'-Trihydroxyacetophenone
	4-Acetylpyrogallol
	1-(2,3,4-Trihydroxyphenyl)ethanone
	NSC 66553
Inchi:	InChI=1S/C8H8O4/c1-4(9)5-2-3-6(10)8(12)7(5)11/h2-3,10-12H,1H3
InchiKey:	XIROXSOOOAZHLL-UHFFFAOYSA-N
Formula:	C8H8O4
SMILES:	CC(=O)c1ccc(O)c(O)c1O
Mol. weight [g/mol]:	168.15
CAS:	528-21-2

Physical Properties

Property code	Value	Unit	Source
gf	-463.89	kJ/mol	Joback Method
hf	-616.43	kJ/mol	Joback Method
hfus	29.46	kJ/mol	Joback Method
hvap	81.47	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	1.006		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
pc	7627.62	kPa	Joback Method
tb	704.85	K	Joback Method
tc	958.07	K	Joback Method
tf	591.43	K	Joback Method
vc	0.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.57	J/mol×K	704.85	Joback Method
cpg	322.12	J/mol×K	747.05	Joback Method
cpg	329.41	J/mol×K	789.26	Joback Method
cpg	336.67	J/mol×K	831.46	Joback Method
cpg	344.12	J/mol×K	873.67	Joback Method
cpg	351.99	J/mol×K	915.87	Joback Method
cpg	360.50	J/mol×K	958.07	Joback Method
dvisc	0.0000027	Pa×s	591.43	Joback Method
dvisc	0.0000017	Pa×s	610.33	Joback Method
dvisc	0.0000011	Pa×s	629.24	Joback Method
dvisc	0.0000007	Pa×s	648.14	Joback Method
dvisc	0.0000005	Pa×s	667.04	Joback Method
dvisc	0.0000003	Pa×s	685.95	Joback Method
dvisc	0.0000002	Pa×s	704.85	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C528212&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume