

Acetophenone, 2,4,5-trihydroxy

Inchi:	InChI=1S/C8H8O4/c1-4(9)5-2-7(11)8(12)3-6(5)10/h2-3,10-12H,1H3
InchiKey:	WCJLAYDOJJYRHF-UHFFFAOYSA-N
Formula:	C8H8O4
SMILES:	CC(=O)c1cc(O)c(O)cc1O
Mol. weight [g/mol]:	168.15
CAS:	1818-27-5

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/molxK	704.85	Joback Method
cpg	351.99	J/molxK	915.87	Joback Method
cpg	344.12	J/molxK	873.67	Joback Method
cpg	336.67	J/molxK	831.46	Joback Method
cpg	329.41	J/molxK	789.26	Joback Method
cpg	322.12	J/molxK	747.05	Joback Method
cpg	360.50	J/molxK	958.07	Joback Method
dvisc	0.0000002	Paxs	704.85	Joback Method
dvisc	0.0000003	Paxs	685.95	Joback Method

dvisc	0.0000005	Paxs	667.04	Joback Method
dvisc	0.0000007	Paxs	648.14	Joback Method
dvisc	0.0000011	Paxs	629.24	Joback Method
dvisc	0.0000017	Paxs	610.33	Joback Method
dvisc	0.0000027	Paxs	591.43	Joback Method

Sources

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=C1818275&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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