2',4'-Dihydroxy-3'-methylacetophenone

Other names: 1-(2,4-Dihydroxy-3-methylphenyl)ethanone
Inchi: InChI=1S/C9H10O3/c1-5-8(11)4-3-7(6(2)10)9(5)12/h3-4,11-12H,1-2H3
InchiKey: KMTLZBUHQPQFAV-UHFFFAOYSA-N
Formula: C9H10O3
SMILES: CC(=O)c1ccc(O)c(C)c1O
Mol. weight [g/mol]: 166.17
CAS: 10139-84-1

Physical Properties

Property code	Value	Unit	Source
gf	-310.48	kJ/mol	Joback Method
hf	-471.23	kJ/mol	Joback Method
hfus	25.88	kJ/mol	Joback Method
hvap	71.34	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.609		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	5065.79	kPa	Joback Method
ripol	1893.00		NIST Webbook
ripol	1893.00		NIST Webbook
tb	652.09	K	Joback Method
tc	893.33	K	Joback Method
tf	503.50	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.95	J/mol×K	652.09	Joback Method
cpg	332.56	J/mol×K	692.30	Joback Method
cpg	341.55	J/mol×K	732.50	Joback Method
cpg	350.07	J/mol×K	772.71	Joback Method
cpg	358.26	J/mol×K	812.91	Joback Method
cpg	366.25	J/mol×K	853.12	Joback Method

cpg	374.17	J/mol×K	893.33	Joback Method
dvisc	0.0000729	Pa×s	503.50	Joback Method
dvisc	0.0000401	Pa×s	528.26	Joback Method
dvisc	0.0000233	Pa×s	553.03	Joback Method
dvisc	0.0000142	Pa×s	577.80	Joback Method
dvisc	0.0000090	Pa×s	602.56	Joback Method
dvisc	0.0000059	Pa×s	627.33	Joback Method
dvisc	0.0000040	Pa×s	652.09	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10139841&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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