1-Butanone, 1-(2,4,5-trihydroxyphenyl)-

Other names:	Butyrophenone, 2',4',5'-trihydroxy-
	THBP
	2,4,5-Trihydroxybutyrophenone
	2',4',5'-Trihydroxybutyrophenone
	USAF EK
	1-(2,4,5-Trihydroxyphenyl)-1-butanone
	NSC 73478
Inchi:	InChI=1S/C10H12O4/c1-2-3-7(11)6-4-9(13)10(14)5-8(6)12/h4-5,12-14H,2-3H2,1H3
InchiKey:	SRUQARLMFOLRDN-UHFFFAOYSA-N
Formula:	C10H12O4
SMILES:	CCCC(=O)c1cc(O)c(O)cc1O
Mol. weight [g/mol]:	196.20
CAS:	1421-63-2

Physical Properties

Property code	Value	Unit	Source
gf	-447.05	kJ/mol	Joback Method
hf	-657.71	kJ/mol	Joback Method
hfus	34.64	kJ/mol	Joback Method
hvap	85.92	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.786		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	5594.19	kPa	Joback Method
tb	750.61	K	Joback Method
tc	993.14	K	Joback Method
tf	613.97	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.30	J/mol×K	750.61	Joback Method
cpg	460.40	J/mol×K	952.72	Joback Method

cpg	450.34	J/mol×K	912.29	Joback Method
cpg	440.71	J/mol×K	871.87	Joback Method
cpg	431.29	J/mol×K	831.45	Joback Method
cpg	421.90	J/mol×K	791.03	Joback Method
cpg	471.10	J/mol×K	993.14	Joback Method
dvisc	0.0000001	Pa×s	750.61	Joback Method
dvisc	0.0000002	Pa×s	727.84	Joback Method
dvisc	0.0000002	Pa×s	705.06	Joback Method
dvisc	0.0000004	Pa×s	682.29	Joback Method
dvisc	0.0000006	Pa×s	659.52	Joback Method
dvisc	0.0000010	Pa×s	636.74	Joback Method
dvisc	0.0000016	Pa×s	613.97	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=C1421632&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