Benzyl 2,4-Dihydroxyphenyl ketone

Other names: Ethanone, 1-(2,4-dihydroxyphenyl)-2-phenyl-
Inchi: InChI=1S/C14H12O3/c15-11-6-7-12(14(17)9-11)13(16)8-10-4-2-1-3-5-10/h1-7,9,15,17H,
InchiKey: VFQKAJVKZKHVPD-UHFFFAOYSA-N
Formula: C14H12O3
SMILES: O=C(Cc1ccccc1)c1ccc(O)cc1O
Mol. weight [g/mol]: 228.25

Physical Properties

Property code	Value	Unit	Source
hf	-325.95	kJ/mol	Cheméo Relay (1.0)
hfus	33.26	kJ/mol	Joback Method
hvap	116.15	kJ/mol	Cheméo Relay (1.0)
ie	8.00	eV	Cheméo Relay (1.0)
log10ws	-3.17		Cheméo Relay (1.0)
logp	2.523		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
tb	630.51	K	Cheméo Relay (1.0)
tf	416.68	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.38	J/mol×K	788.19	Joback Method
cpg	495.23	J/mol×K	831.54	Joback Method
cpg	506.55	J/mol×K	874.89	Joback Method
cpg	517.59	J/mol×K	918.24	Joback Method
cpg	528.56	J/mol×K	961.59	Joback Method
cpg	539.69	J/mol×K	1004.94	Joback Method
cpg	551.22	J/mol×K	1048.29	Joback Method
dvisc	0.0000210	Pa×s	573.75	Joback Method
dvisc	0.0000103	Pa×s	609.49	Joback Method
dvisc	0.0000055	Pa×s	645.23	Joback Method
dvisc	0.0000031	Pa×s	680.97	Joback Method

dvisc	0.0000019	Pa×s	716.71	Joback Method
dvisc	0.0000012	Pa×s	752.45	Joback Method
dvisc	0.0000008	Pa×s	788.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3669418&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point