

2,4-Dihydroxyphenylbenzyl 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]:	228.24
CAS:	3669-41-8

Physical Properties

Property code	Value	Unit	Source
gf	-146.34	kJ/mol	Joback Method
hf	-326.43	kJ/mol	Joback Method
hfus	33.26	kJ/mol	Joback Method
hvap	84.08	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.523		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
tb	788.19	K	Joback Method
tc	1048.29	K	Joback Method
tf	573.75	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.38	J/molxK	788.19	Joback Method
cpg	495.23	J/molxK	831.54	Joback Method
cpg	506.55	J/molxK	874.89	Joback Method
cpg	517.59	J/molxK	918.24	Joback Method
cpg	528.56	J/molxK	961.59	Joback Method
cpg	539.69	J/molxK	1004.94	Joback Method
cpg	551.22	J/molxK	1048.29	Joback Method
dvisc	0.0000210	Paxs	573.75	Joback Method

dvisc	0.0000103	Paxs	609.49	Joback Method
dvisc	0.0000055	Paxs	645.23	Joback Method
dvisc	0.0000031	Paxs	680.97	Joback Method
dvisc	0.0000019	Paxs	716.71	Joback Method
dvisc	0.0000012	Paxs	752.45	Joback Method
dvisc	0.0000008	Paxs	788.19	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=C3669418&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ 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

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