2-Butanone, 4-(4-hydroxyphenyl)-

Other names:	(p-Hydroxybenzyl)acetone
	1-(4-Hydroxyphenyl)-3-butanone
	1-(p-Hydroxyphenyl)-3-butanone
	2-Butanone, 4-(p-hydroxyphenyl)-
	4-(3-Oxobutyl)phenol
	4-(4-Hydroxyphenyl)-2-butanone
	4-(4-hydroxyphenyl)butan-2-one
	4-(p-Hydroxyphenyl)-2-butanone
	4-Hydroxybenzylacetone
	Frambinone
	NSC 26515
	Oxyphenalon
	Rheosmin
	raspberry ketone
Inchi:	InChI=1S/C10H12O2/c1-8(11)2-3-9-4-6-10(12)7-5-9/h4-7,12H,2-3H2,1H3
InchiKey:	NJGBTKGETPDVIK-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC(=O)CCc1ccc(O)cc1
Mol. weight [g/mol]:	164.20
CAS:	5471-51-2

Physical Properties

Property code	Value	Unit	Source
gf	-137.81	kJ/mol	Joback Method
hf	-303.09	kJ/mol	Joback Method
hfus	23.08	kJ/mol	Joback Method
hvap	59.89	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.914		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
rinpol	1498.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1490.00		NIST Webbook

rinpol	1554.00		NIST Webbook
ripol	2952.00		NIST Webbook
ripol	2982.00		NIST Webbook
ripol	3000.00		NIST Webbook
ripol	2970.00		NIST Webbook
ripol	3000.00		NIST Webbook
tb	589.37	K	Joback Method
tc	815.81	K	Joback Method
tf	355.00	K	Solubility Determination and Modeling and Dissolution Thermodynamic Properties of Raspberry Ketone in Binary Solvent Mixtures of Ethanol andWater
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.20	J/mol×K	589.37	Joback Method
cpg	381.12	J/mol×K	778.07	Joback Method
cpg	371.74	J/mol×K	740.33	Joback Method
cpg	361.74	J/mol×K	702.59	Joback Method
cpg	351.04	J/mol×K	664.85	Joback Method
cpg	339.55	J/mol×K	627.11	Joback Method
cpg	389.96	J/mol×K	815.81	Joback Method
dvisc	0.0000452	Pa×s	589.37	Joback Method
dvisc	0.0000681	Pa×s	556.23	Joback Method
dvisc	0.0001079	Pa×s	523.09	Joback Method
dvisc	0.0001821	Pa×s	489.95	Joback Method
dvisc	0.0003314	Pa×s	456.81	Joback Method
dvisc	0.0006624	Pa×s	423.67	Joback Method
dvisc	0.0014890	Pa×s	390.53	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Solubility Determination and Modeling and Dissolution Thermodynamic Properties of Raspberry Ketone in Binary Solvent Mixtures of Ethanol andWater.	https://www.doi.org/10.1007/s10765-017-2323-6
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=C5471512&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume