4-(O-hydroxyphenyl)-3-buten-2-one

Other names: 4-(2-hydroxyphenyl)but-3-en-2-one
Inchi: InChI=1S/C10H10O2/c1-8(11)6-7-9-4-2-3-5-10(9)12/h2-7,12H,1H3/b7-6+
InchiKey: OIKUPYQBJLSNAS-VOTSOKGWSA-N
Formula: C10H10O2
SMILES: CC(=O)C=Cc1ccccc1O
Mol. weight [g/mol]: 162.19
CAS: 6051-53-2

Physical Properties

Property code	Value	Unit	Source
gf	-57.59	kJ/mol	Joback Method
hf	-185.87	kJ/mol	Joback Method
hfus	23.28	kJ/mol	Joback Method
hvap	59.85	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.994		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	593.53	K	Joback Method
tc	830.21	K	Joback Method
tf	385.45	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.69	J/mol×K	593.53	Joback Method
cpg	356.82	J/mol×K	790.76	Joback Method
cpg	348.17	J/mol×K	751.32	Joback Method
cpg	338.95	J/mol×K	711.87	Joback Method
cpg	329.04	J/mol×K	672.42	Joback Method
cpg	318.32	J/mol×K	632.98	Joback Method
cpg	365.00	J/mol×K	830.21	Joback Method
dvisc	0.0000375	Pa×s	593.53	Joback Method

dvisc	0.0000572	Pa×s	558.85	Joback Method
dvisc	0.0000920	Pa×s	524.17	Joback Method
dvisc	0.0001584	Pa×s	489.49	Joback Method
dvisc	0.0002964	Pa×s	454.81	Joback Method
dvisc	0.0006148	Pa×s	420.13	Joback Method
dvisc	0.0014544	Pa×s	385.45	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=C6051532&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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