Ethanone, 1-[4-(1-hydroxy-1-methylethyl)phenyl]-

Other names: 1-[4-(1-Hydroxy-1-methylethyl)phenyl]ethanone
Inchi: InChI=1S/C11H14O2/c1-8(12)9-4-6-10(7-5-9)11(2,3)13/h4-7,13H,1-3H3
InchiKey: KWWWFTBWCKTBQI-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: CC(=O)c1ccc(C(C)(C)O)cc1
Mol. weight [g/mol]: 178.23
CAS: 54549-72-3

Physical Properties

Property code	Value	Unit	Source
gf	-118.38	kJ/mol	Joback Method
hf	-318.87	kJ/mol	Joback Method
hfus	16.17	kJ/mol	Joback Method
hvap	65.15	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.117		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
rinpol	1432.00		NIST Webbook
tb	625.56	K	Joback Method
tc	834.96	K	Joback Method
tf	365.84	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.05	J/mol×K	625.56	Joback Method
cpg	431.83	J/mol×K	800.06	Joback Method
cpg	422.54	J/mol×K	765.16	Joback Method
cpg	412.56	J/mol×K	730.26	Joback Method
cpg	401.85	J/mol×K	695.36	Joback Method
cpg	390.37	J/mol×K	660.46	Joback Method
cpg	440.50	J/mol×K	834.96	Joback Method

dvisc	0.0000671	Pa×s	625.56	Joback Method
dvisc	0.0001021	Pa×s	582.27	Joback Method
dvisc	0.0001663	Pa×s	538.99	Joback Method
dvisc	0.0002948	Pa×s	495.70	Joback Method
dvisc	0.0005832	Pa×s	452.41	Joback Method
dvisc	0.0013330	Pa×s	409.13	Joback Method
dvisc	0.0037049	Pa×s	365.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54549723&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume