

1-Hydroxy-1-(4-methoxyphenyl)propan-2-one

InChI: InChI=1S/C10H12O3/c1-7(11)10(12)8-3-5-9(13-2)6-4-8/h3-6,10,12 H,1-2H3

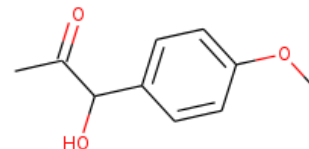
InChI Key: UVVXGUZSUNRWQG-UHFFFAOYSA-N

Formula: C10H12O3

SMILES: COc1ccc(C(O)C(C)=O)cc1

Molecular Weight: 180.20

CAS: 15482-29-8



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-237.08	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-426.98	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	18.66	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	66.24	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.32		Crippen Method
P_c	3395.98	kPa	Joback Method
T_{boil}	627.89	K	Joback Method
T_c	831.09	K	Joback Method
T_{fus}	359.38	K	Joback Method
V_c	0.52	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	350.72	J/mol×K	627.89	Joback Method
η	0.00	Paxs	627.89	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H12O3/c1-7\(11\)10\(12\)8-3-5-9\(13-2\)6-4-8/h3-6,10,12H,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H12O3/c1-7(11)10(12)8-3-5-9(13-2)6-4-8/h3-6,10,12H,1-2H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/molxK).

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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