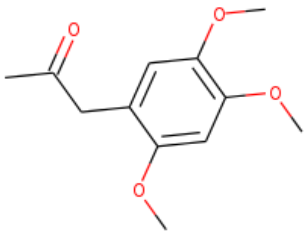
1-(2,4,5-Trimethoxyphenyl)propan-2-one

InChI: InChI=1S/C12H16O4/c1-8(13)5-9-6-11(15-3)12(16-4)7-10(9)14-2/h6-7H,5H2,1-4H3
InChI Key: AQZHZTTUVYQMIN-UHFFFAOYSA-N
Formula: C12H16O4
SMILES: COc1cc(OC)c(OC)cc1CC(C)=O
Molecular Weight: 224.25
CAS: 2020-90-8



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-310.24	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-598.13	kJ/mol	Joback Method
$\Delta_{fus} H°$	24.87	kJ/mol	Joback Method
$\Delta_{vap} H°$	60.54	kJ/mol	Joback Method
$logP_{oct/wat}$	1.84		Crippen Method
P_c	2329.27	kPa	Joback Method
T_{boil}	636.71	K	Joback Method
T_c	841.45	K	Joback Method
T_{fus}	405.60	K	Joback Method
V_c	0.66	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	443.68	J/mol×K	636.71	Joback Method
η	0.00	Pa×s	636.71	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H16O4/c1-8(13)5-9-6-11(15-3)12(16-4)7-10(9)14-2/h6-7H,5H2,1-4H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).