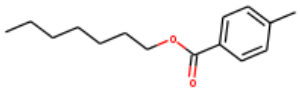
p-Toluic acid, heptyl ester

Other names: p-Toluylic acid, heptyl ester.
InChI: InChI=1S/C15H22O2/c1-3-4-5-6-7-12-17-15(16)14-10-8-13(2)9-11-14/h8-11H,3-7,12H2,1-2H3
InChI Key: XPCXKYHMNRJMRA-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CCCCCCCOC(=O)c1ccc(C)cc1
Molecular Weight: 234.33
CAS: 331810-92-5



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-55.72	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-372.67	kJ/mol	Joback Method
$\Delta_{fus} H°$	31.04	kJ/mol	Joback Method
$\Delta_{vap} H°$	61.08	kJ/mol	Joback Method
$logP_{oct/wat}$	4.12		Crippen Method
P_c	1896.95	kPa	Joback Method
T_{boil}	650.55	K	Joback Method
T_c	848.93	K	Joback Method
T_{fus}	369.91	K	Joback Method
V_c	0.79	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	546.11	J/mol×K	650.55	Joback Method
η	0.00	Pa×s	650.55	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H22O2/c1-3-4-5-6-7-12-17-15(16)14-10-8-13(2)9-11-14/h8-11H,3-7,12H2,1-2H3
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).