3-Cyclopentylpropionic acid, 3,5-dimethylphenyl ester

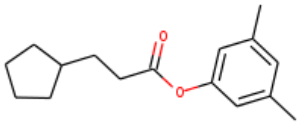
InChI: InChI=1S/C16H22O2/c1-12-9-13(2)11-15(10-12)18-16(17)8-7-14-5-3-4-6-14/h9-11,14H,3-8H2,1-2H3

InChI Key: OKDQBRBJEFQPGL-UHFFFAOYSA-N

Formula: C16H22O2

SMILES: Cc1cc(C)cc(OC(=O)CCC2CCCC2)c1

Molecular Weight: 246.34



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-20.38	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-344.30	kJ/mol	Joback Method
$\Delta_{fus} H°$	27.18	kJ/mol	Joback Method
$\Delta_{vap} H°$	64.22	kJ/mol	Joback Method
$logP_{oct/wat}$	4.18		Crippen Method
P_c	2016.32	kPa	Joback Method
T_{boil}	693.69	K	Joback Method
T_c	914.87	K	Joback Method
T_{fus}	404.60	K	Joback Method
V_c	0.79	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	590.10	J/mol×K	693.69	Joback Method
η	0.00	Pa×s	693.69	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H22O2/c1-12-9-13(2)11-15(10-12)18-16(17)8-7-14-5-3-4-6-14/h9-11,14H,3-8H2,1-2H3
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).