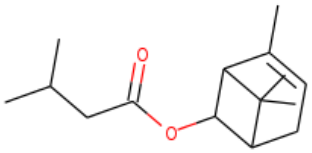
Chrysanthenyl isovalerate

InChI: InChI=1S/C15H24O2/c1-9(2)8-12(16)17-14-11-7-6-10(3)13(14)15(11,4)5/h6,9,11,13-14H,7-8H2,1-5H3
InChI Key: VCFDIPBWQNPUTA-UHFFFAOYSA-N
Formula: C15H24O2
SMILES: CC1=CCC2C(OC(=O)CC(C)C)C1C2(C)C
Molecular Weight: 236.35



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-52.12	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-442.70	kJ/mol	Joback Method
$\Delta_{fus} H°$	24.72	kJ/mol	Joback Method
$\Delta_{vap} H°$	56.94	kJ/mol	Joback Method
$logP_{oct/wat}$	3.567		Crippen Method
P_c	1859.51	kPa	Joback Method
T_{boil}	631.24	K	Joback Method
T_c	836.07	K	Joback Method
T_{fus}	377.03	K	Joback Method
V_c	0.781	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	574.62	J/mol×K	631.24	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H24O2/c1-9(2)8-12(16)17-14-11-7-6-10(3)13(14)15(11,4)5/h6,9,11,13-14H,7-8H2,1-5H3

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: 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).

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