ent-manoyl oxide

Other names: -manoyl-oxide.

InChI: InChI=1S/C20H34O/c1-7-18(4)13-9-16-19(5)12-8-11-17(2,3)15(19)10-14-20(16,6)21-18/h7,15-16H,1,8-14H2,2-6H3/t15?,16?,18-,19-,20+/m1/s1

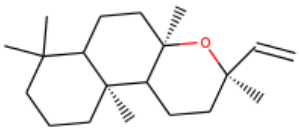
InChI Key: IGGWKHQYMAJOHK-XZJNCXDESA-N

Formula: C20H34O

SMILES: C=CC1(C)CCC2C(C)(CCC3C(C)(C)CCCC32C)O1

Molecular Weight: 290.48

CAS: 27642-41-7



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	195.90	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-275.16	kJ/mol	Joback Method
$\Delta_{fus} H°$	16.18	kJ/mol	Joback Method
$\Delta_{vap} H°$	59.02	kJ/mol	Joback Method
$logP_{oct/wat}$	5.74		Crippen Method
P_c	1588.54	kPa	Joback Method
T_{boil}	709.15	K	Joback Method
T_c	951.08	K	Joback Method
T_{fus}	459.07	K	Joback Method
V_c	0.98	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	821.83	J/mol×K	709.15	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H34O/c1-7-18(4)13-9-16-19(5)12-8-11-17(2,3)15(19)10-14-20(16,6)21-18/h7,15-16H,1,8-14H2,2-6H3/t15?,16?,18-,19-,20+/m1/s1

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

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*$P_{oct/wat}$**: 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 (m^3/kg-mol).