GA25, Me

Other names: GA25 methyl ester.

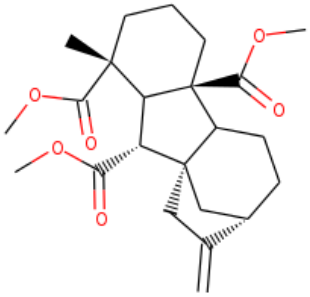
InChI: InChI=1S/C23H32O6/c1-13-11-22-12-14(13)7-8-15(22)23(20(26)29-5)10-6-9-21(2,19(25)28-4)17(23)16(22)18(24)27-3/h14-17H,1,6-12H2,2-5H3/t14-,15?,16-,17?,21-,22+,23-/m1/s1

InChI Key: CVVOOYMCPNGYQG-RXILWBLMSA-N

Formula: C23H32O6

SMILES: C=C1CC23CC1CCC2C1(C(=O)OC)CCCC(C)(C(=O)OC)C1C3C(=O)OC

Molecular Weight: 404.50



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-338.80	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-910.79	kJ/mol	Joback Method
$\Delta_{fus} H°$	33.09	kJ/mol	Joback Method
$\Delta_{vap} H°$	90.21	kJ/mol	Joback Method
$logP_{oct/wat}$	3.291		Crippen Method
P_c	1436.98	kPa	Joback Method
T_{boil}	980.15	K	Joback Method
T_c	1216.30	K	Joback Method
T_{fus}	699.31	K	Joback Method
V_c	1.175	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1147.01	J/mol×K	980.15	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H32O6/c1-13-11-22-12-14(13)7-8-15(22)23(20(26)29-5)10-6-9-21(2,19(25)28-4)17(23)16(22)18(24)27-3/h14-17H,1,6-12H2,2-5H3/t14-,15?,16-,17?,21-,22+,23-/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).