6-Methoxy-2,7,8-trimethyl-2-(4,8,12-trimethyltridecyl)chroman

InChI: InChI=1S/C29H50O2/c1-21(2)12-9-13-22(3)14-10-15-23(4)16-11-18-29(7)19-17-26-20-27(30-8)24(5)25(6)28(26)31-29/h20-23H,9-19H2,1-8H3

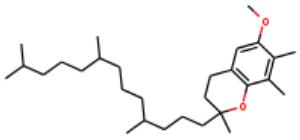
InChI Key: YCYZEPRIDWTCRQ-UHFFFAOYSA-N

Formula: C29H50O2

SMILES: COc1cc2c(c(C)c1C)OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2

Molecular Weight: 430.71

CAS: 79306-82-4



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	111.91	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-649.42	kJ/mol	Joback Method
$\Delta_{fus} H°$	51.69	kJ/mol	Joback Method
$\Delta_{vap} H°$	89.76	kJ/mol	Joback Method
$logP_{oct/wat}$	8.83		Crippen Method
P_c	801.15	kPa	Joback Method
T_{boil}	968.82	K	Joback Method
T_c	1186.68	K	Joback Method
T_{fus}	535.21	K	Joback Method
V_c	1.52	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1391.28	J/mol×K	968.82	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C29H50O2/c1-21(2)12-9-13-22(3)14-10-15-23(4)16-11-18-29(7)19-17-26-20-27(30-8)24(5)25(6)28(26)31-29/h20-23H,9-19H2,1-8H3

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).