cis-3,6,9,12,15-heneicosapentaene

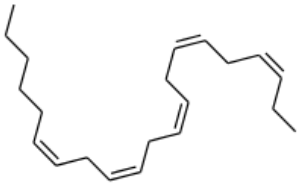
InChI: InChI=1S/C21H34/c1-3-5-7-9-11-13-15-17-19-21-20-18-16-14-12-10-8-6-4-2/h5,7,11-14,17-20H,3-4,6,8-10,15-16,21H2,1-2H3/b7-5-,13-11-,14-12-,19-17-,20-18-

InChI Key: WVVMNHZOUMNOLT-LOYOHVQTSA-N

Formula: C21H34

SMILES: CCC=CCC=CCC=CCC=CCC=CCCCCC

Molecular Weight: 286.49



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	527.04	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	109.33	kJ/mol	Joback Method
$\Delta_{fus} H°$	51.16	kJ/mol	Joback Method
$\Delta_{vap} H°$	62.13	kJ/mol	Joback Method
$logP_{oct/wat}$	7.32		Crippen Method
P_c	1130.62	kPa	Joback Method
T_{boil}	700.68	K	Joback Method
T_c	883.89	K	Joback Method
T_{fus}	301.03	K	Joback Method
V_c	1.11	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	792.26	J/mol×K	700.68	Joback Method
η	0.00	Pa×s	700.68	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H34/c1-3-5-7-9-11-13-15-17-19-21-20-18-16-14-12-10-8-6-4-2/h5,7,11-14,17-20H,3-4,6,8-10,15-16,21H2,1-2H3/b7-5-,13-11-,14-12-,19-17-,20-18-
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f G°$: 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).