Chrysene, octadecahydro-

Other names: Chrysitane; D-Homo-18-norestrane; Octadecahydrochrysene; Perhydrochrysene; Perhydrochrysene, # 1; Perhydrochrysene, # 2; Perhydrochrysene, # 3; Perhydrochrysene, # 4; Perhydrochrysene, # 5; Perhydrochrysene, # 6; Perhydrochrysene, # 7.

InChI: InChI=1S/C18H30/c1-3-7-15-13(5-1)9-11-18-16-8-4-2-6-14(16)10-12-17(15)18/h13-18H,1-12H2

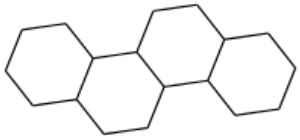
InChI Key: ZEMKTMFBYLHVNN-UHFFFAOYSA-N

Formula: C18H30

SMILES: C1CCC2C(C1)CCC1C3CCCCC3CCC21

Molecular Weight: 246.43

CAS: 2090-14-4



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	255.66	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-201.29	kJ/mol	Joback Method
$\Delta_{fus} H°$	24.46	kJ/mol	Joback Method
$\Delta_{vap} H°$	55.73	kJ/mol	Joback Method
$log P_{oct/wat}$	5.42		Crippen Method
P_c	1823.17	kPa	Joback Method
T_{boil}	654.48	K	Joback Method
T_c	892.74	K	Joback Method
T_{fus}	334.78	K	Joback Method
V_c	0.82	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	693.36	J/mol×K	654.48	Joback Method
η	0.00	Pa×s	654.48	Joback Method
$\Delta_{vap} H$	82.40	kJ/mol	313.0	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H30/c1-3-7-15-13(5-1)9-11-18-16-8-4-2-6-14(16)10-12-17(15)18/h13-18H,1-12H2
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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