

Phenanthrene, tetradecahydro-4,5-dimethyl-

Other names: 1,3-dimethyltricyclo[8.4.0.0(2,6)]tetradecane.

InChI: InChI=1S/C16H28/c1-11-5-3-7-13-9-10-14-8-4-6-12(2)16(14)15(11)13/h11-16H,3-10H2,1-2H3

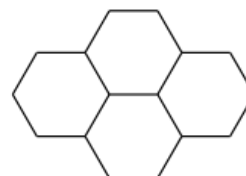
InChI Key: LRCLMXSQZAMLRU-UHFFFAOYSA-N

Formula: C₁₆H₂₈

SMILES: CC1CCCC2CCC3CCCC(C)C3C12

Molecular Weight: 220.39

CAS: 56292-68-3



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	182.46	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-246.99	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	24.31	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	50.88	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.89		Crippen Method
P_c	1829.41	kPa	Joback Method
T_{boil}	593.04	K	Joback Method
T_c	816.70	K	Joback Method
T_{fus}	293.58	K	Joback Method
V_c	0.76	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	587.04	J/mol×K	593.04	Joback Method
η	0.00	Paxs	593.04	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H28/c1-11-5-3-7-13-9-10-14-8-4-6-12\(2\)16\(14\)15\(11\)13/h11-16H,3-10H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H28/c1-11-5-3-7-13-9-10-14-8-4-6-12(2)16(14)15(11)13/h11-16H,3-10H2,1-2H3)

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

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/molxK).

η : Dynamic viscosity (Pa.s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: 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 (m³/kg-mol).

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