1,4:5,8:9,10-Trimethanoanthracene, 1,2,3,4,4a,5,8,8a,9,9a,10,10a-dodecahydro-(1«alpha»,4«alpha»,4a«beta»,5«beta»,8«beta»,8a«beta»,9«alpha»,9a«beta»,10«alpha»,10a«beta»)-

InChI: InChI=1S/C17H22/c1-2-9-5-8(1)14-12-7-13(15(9)14)17-11-4-3-10(6-11)16(12)17/h1-2,8-17H,3-7H2/t8-,9+,10-,11+,12+,13-,14-,15+,16+,17-

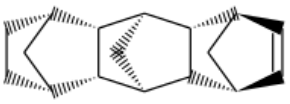
InChI Key: FUCGLOJSPSEIKX-DTSMLRQCSA-N

Formula: C17H22

SMILES: C1=CC2CC1C1C3CC(C21)C1C2CCC(C2)C31

Molecular Weight: 226.36

CAS: 87480-43-1



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	467.98	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	25.17	kJ/mol	Joback Method
$\Delta_{fus} H°$	36.20	kJ/mol	Joback Method
$\Delta_{vap} H°$	51.80	kJ/mol	Joback Method
IE	8.47	eV	NIST Webbook
$logP_{oct/wat}$	3.74		Crippen Method
P_c	2083.12	kPa	Joback Method
T_{boil}	605.01	K	Joback Method
T_c	828.43	K	Joback Method
T_{fus}	376.31	K	Joback Method
V_c	0.72	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	569.82	J/mol×K	605.01	Joback Method

Property	Value	Unit	Temperature (K)	Source
η	0.06	Pa×s	605.01	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H22/c1-2-9-5-8(1)14-12-7-13(15(9)14)17-11-4-3-10(6-11)16(12)17/h1-2,8-17H,3-7H2/t8-,9+,10-,11+,12+,13-,14-,15+,16+,17-

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).
IE: Ionization energy (eV).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: 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).