

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-

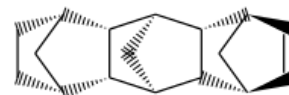
InChI Key: FUCGLOJSPSEIKX-DTSMRLRQCSA-N

Formula: C17H22

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

Molecular Weight: 226.36

CAS: 87480-43-1



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	467.98	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	25.17	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	36.20	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	51.80	kJ/mol	Joback Method
IE	8.47	eV	NIST Webbook
$\log P_{\text{oct/wat}}$	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
$C_{p,\text{gas}}$	569.82	J/molxK	605.01	Joback Method

Property	Value	Unit	Temperature (K)	Source
η	0.06	Paxs	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-](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/ci9903071>

Legend

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

η : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$: 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).

IE: Ionization energy (eV).

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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