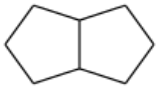
trans-Bicyclo[3.3.0]octane

InChI: InChI=1S/C8H14/c1-3-7-5-2-6-8(7)4-1/h7-8H,1-6H2/t7-,8-
InChI Key: AEBWATHAIVJLTA-ZKCHVHJHSA-N
Formula: C8H14
SMILES: C1CC2CCCC2C1
Molecular Weight: 110.20
CAS: 5597-89-7



Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{liquid}$	-5040.00 ± 2.00	kJ/mol	NIST Webbook
$\Delta_c H°_{liquid}$	-5041.70 ± 5.00	kJ/mol	NIST Webbook
$\Delta_f G°$	113.78	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-67.00 ± 3.00	kJ/mol	NIST Webbook
$\Delta_f H°_{liquid}$	-109.00 ± 2.00	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	8.55	kJ/mol	Joback Method
$\Delta_{vap} H°$	42.70 ± 0.80	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	42.00	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	42.70 ± 0.80	kJ/mol	NIST Webbook
$log P_{oct/wat}$	2.59		Crippen Method
P_c	3560.02	kPa	Joback Method
T_{boil}	405.00 ± 2.00	K	NIST Webbook
T_{boil}	409.40 ± 2.00	K	NIST Webbook
T_{boil}	407.00 ± 3.00	K	NIST Webbook
T_{boil}	405.00 ± 3.00	K	NIST Webbook
T_{boil}	405.20	K	NIST Webbook
T_c	614.38	K	Joback Method

Property	Value	Unit	Source
T_{fus}	243.00 ± 3.00	K	NIST Webbook
T_{fus}	244.00 ± 3.00	K	NIST Webbook
T_{fus}	237.00 ± 3.00	K	NIST Webbook
V_c	0.38	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	198.70	J/mol×K	404.46	Joback Method
$C_{p,liquid}$	180.30	J/mol×K	308.0	NIST Webbook
η	0.00	Pa×s	404.46	Joback Method
$\Delta_{vap}H$	41.40	kJ/mol	309.0	NIST Webbook
$\Delta_{vap}H$	41.30 ± 0.40	kJ/mol	320.0	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H14/c1-3-7-5-2-6-8(7)4-1/h7-8H,1-6H2/t7-,8-
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\Delta_c H°_{liquid}$: Standard liquid enthalpy of combustion (kJ/mol).
$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$C_{p,liquid}$: Liquid phase 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).
$\Delta_f H°_{liquid}$: Liquid phase 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).
$\Delta_{vap} H$: Enthalpy of vaporization at a given temperature (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 (m^3/kg-mol).