

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-

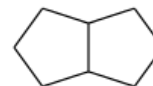
InChI Key: AEBWATHAIVJLTA-ZKCHVHJHSA-N

Formula: C8H14

SMILES: C1CC2CCCC2C1

Molecular Weight: 110.20

CAS: 5597-89-7



Physical Properties

Property	Value	Unit	Source
$\Delta_c H^\circ_{\text{liquid}}$	-5040.00 \pm 2.00	kJ/mol	NIST Webbook
$\Delta_c H^\circ_{\text{liquid}}$	-5041.70 \pm 5.00	kJ/mol	NIST Webbook
$\Delta_f G^\circ$	113.78	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-67.00 \pm 3.00	kJ/mol	NIST Webbook
$\Delta_f H^\circ_{\text{liquid}}$	-109.00 \pm 2.00	kJ/mol	NIST Webbook
$\Delta_{\text{fus}} H^\circ$	8.55	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	42.70 \pm 0.80	kJ/mol	NIST Webbook
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$\log P_{\text{oct/wat}}$	2.587		Crippen Method
P_c	3560.02	kPa	Joback Method
T_{boil}	405.00 \pm 2.00	K	NIST Webbook
T_{boil}	409.40 \pm 2.00	K	NIST Webbook
T_{boil}	407.00 \pm 3.00	K	NIST Webbook
T_{boil}	405.00 \pm 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}	0.382	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{\text{p,gas}}$	198.70	J/mol×K	404.46	Joback Method
$C_{\text{p,liquid}}$	180.30	J/mol×K	308.0	NIST Webbook
η	0.0004750	Paxs	404.46	Joback Method
$\Delta_{\text{vap}}H$	41.40	kJ/mol	309.0	NIST Webbook
$\Delta_{\text{vap}}H$	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-](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/ci9903071>

Legend

$\Delta_{\text{c}}H^{\circ}_{\text{liquid}}$: Standard liquid enthalpy of combustion (kJ/mol).

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

$C_{\text{p,liquid}}$: Liquid phase heat capacity (J/mol×K).

η : Dynamic viscosity (Paxs).

$\Delta_{\text{f}}G^{\circ}$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_{\text{f}}H^{\circ}_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{f}}H^{\circ}_{\text{liquid}}$: Liquid phase enthalpy of formation at standard conditions (kJ/mol).

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

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

$\Delta_{\text{vap}}H$: Enthalpy of vaporization at a given temperature (kJ/mol).

$\log P_{\text{oct/wat}}$: 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 ($\text{m}^3/\text{kg}\text{-mol}$).

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