6,8-Dioxabicyclo[3.2.1]octane, 7-ethyl-5-methyl-, (1r-exo)-

Other names: Brevicomin;
exo-7-Ethyl-5-methyl-6,8-dioxabicyclo[3.2.1]octane; exo-Brevicomin.

InChI:
InChI=1S/C9H16O2/c1-3-7-8-5-4-6-9(2,10-7)11-8/h7-8H,3-6H2,1-2H3

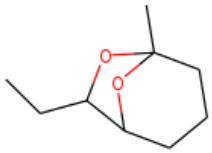
InChI Key: YONXEBYXWVCXIV-UHFFFAOYSA-N

Formula: C9H16O2

SMILES: CCC1OC2(C)CCCC1O2

Molecular Weight: 156.22

CAS: 20290-99-7



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-63.24	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-364.91	kJ/mol	Joback Method
$\Delta_{fus} H°$	21.87	kJ/mol	Joback Method
$\Delta_{vap} H°$	43.36	kJ/mol	Joback Method
$logP_{oct/wat}$	2.08		Crippen Method
P_c	3163.27	kPa	Joback Method
T_{boil}	370.50 ± 2.50	K	NIST Webbook
T_c	691.82	K	Joback Method
T_{fus}	292.83	K	Joback Method
V_c	0.48	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	308.21	J/mol×K	476.81	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H16O2/c1-3-7-8-5-4-6-9(2,10-7)11-8/h7-8H,3-6H2,1-2H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: 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).
$log P_{oct/wat}$: 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).