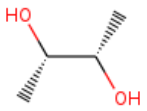
2,3-Butanediol, [S-(R*,R*)]-

Other names: (2S,3S)-(+)-2,3-Butanediol; [S,S]-2,3-butanediol.
InChI: InChI=1S/C4H10O2/c1-3(5)4(2)6/h3-6H,1-2H3/t3-,4-/m1/s1
InChI Key: OWBTYPJTUOEWEK-QWWZWVQMSA-N
Formula: C4H10O2
SMILES: CC(O)C(C)O
Molecular Weight: 90.12
CAS: 19132-06-0



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-295.72	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-440.91	kJ/mol	Joback Method
$\Delta_{fus} H°$	7.25	kJ/mol	Joback Method
$\Delta_{vap} H°$	63.20 ± 0.70	kJ/mol	NIST Webbook
$logP_{oct/wat}$	-0.25		Crippen Method
P_c	5087.49	kPa	Joback Method
T_{boil}	452.70	K	NIST Webbook
T_{boil}	450.00 ± 2.00	K	NIST Webbook
T_c	639.26	K	Joback Method
T_{fus}	293.15 ± 4.00	K	NIST Webbook
V_c	0.29	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	173.55	J/mol×K	474.4	Joback Method
η	0.00	Pa×s	474.4	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C4H10O2/c1-3(5)4(2)6/h3-6H,1-2H3/t3-,4-/m1/s1
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).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: 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).