

1,3-Dioxane, 4,6-dimethyl-, cis-

InChI: InChI=1S/C6H12O2/c1-5-3-6(2)8-4-7-5/h5-6H,3-4H2,1-2H3/t5-,6+

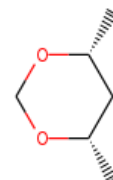
InChI Key: OCBJIXQOIASAQK-OLQVQODUSA-N

Formula: C6H12O2

SMILES: CC1CC(C)OCO1

Molecular Weight: 116.16

CAS: 3390-18-9



Physical Properties

Property	Value	Unit	Source
$\Delta_c H^\circ_{\text{liquid}}$	-3601.30 \pm 2.40	kJ/mol	NIST Webbook
$\Delta_f G^\circ$	-155.86	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-397.19	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{liquid}}$	-474.80 \pm 2.40	kJ/mol	NIST Webbook
$\Delta_{\text{fus}} H^\circ$	20.16	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	38.09	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.16		Crippen Method
P_c	3718.02	kPa	Joback Method
T_{boil}	388.15 \pm 1.50	K	NIST Webbook
T_c	610.20	K	Joback Method
T_{fus}	213.66	K	Joback Method
V_c	0.35	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	193.64	J/mol \times K	405.46	Joback Method

Property	Value	Unit	Temperature (K)	Source
η	0.00	Paxs	405.46	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H12O2/c1-5-3-6\(2\)8-4-7-5/h5-6H,3-4H2,1-2H3/t5-,6+](http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H12O2/c1-5-3-6(2)8-4-7-5/h5-6H,3-4H2,1-2H3/t5-,6+)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\Delta_c H^\circ_{\text{liquid}}$: Standard liquid enthalpy of combustion (kJ/mol).

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

η : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_f H^\circ_{\text{liquid}}$: 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).

$\log P_{\text{oct/wat}}$: 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 (m³/kg-mol).

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