

# (+)-trans-4,5-Bis(iodomethyl)-2,2-dimethyl-1,3-dioxane

<b>Inchi:</b>	InChI=1S/C7H12I2O2/c1-7(2)10-5(3-8)6(4-9)11-7/h5-6H,3-4H2,1-2H3
<b>InchiKey:</b>	WHRBZHCFRKKRJE-UHFFFAOYSA-N
<b>Formula:</b>	C7H12I2O2
<b>SMILES:</b>	CC1(C)OC(CI)C(CI)O1
<b>Mol. weight [g/mol]:</b>	381.98
<b>CAS:</b>	58342-57-7

## Physical Properties

Property code	Value	Unit	Source
gf	-32.30	kJ/mol	Joback Method
hf	-263.03	kJ/mol	Joback Method
hfus	28.43	kJ/mol	Joback Method
hvap	57.43	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.377		Crippen Method
mcvol	162.010	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	605.92	K	Joback Method
tc	876.88	K	Joback Method
tf	364.23	K	Joback Method
vc	0.583	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.58	J/molxK	605.92	Joback Method
cpg	352.92	J/molxK	651.08	Joback Method
cpg	365.33	J/molxK	696.24	Joback Method
cpg	377.02	J/molxK	741.40	Joback Method
cpg	388.24	J/molxK	786.56	Joback Method
cpg	399.22	J/molxK	831.72	Joback Method
cpg	410.17	J/molxK	876.88	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C58342577&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C58342577&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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