

trans 4,5-Dimethyl-1,3-dioxane

Inchi:	InChI=1S/C6H12O2/c1-5-3-7-4-8-6(5)2/h5-6H,3-4H2,1-2H3/t5-,6+/m1/s1
InchiKey:	YMXZGCMNTIZHDC-RITPCOANSA-N
Formula:	C6H12O2
SMILES:	CC1COCOC1C
Mol. weight [g/mol]:	116.16
CAS:	1121-20-6

Physical Properties

Property code	Value	Unit	Source
chl	-3622.80 ± 0.59	kJ/mol	NIST Webbook
gf	-155.86	kJ/mol	Joback Method
hf	-411.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-453.00 ± 1.00	kJ/mol	NIST Webbook
hfus	20.16	kJ/mol	Joback Method
hvap	43.00 ± 1.00	kJ/mol	NIST Webbook
hvap	42.00	kJ/mol	NIST Webbook
log10ws	-0.77		Crippen Method
logp	1.015		Crippen Method
mcvol	96.280	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
tb	405.46	K	Joback Method
tc	610.20	K	Joback Method
tf	213.66	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.89	J/mol×K	610.20	Joback Method
cpg	259.54	J/mol×K	576.08	Joback Method
cpg	247.58	J/mol×K	541.95	Joback Method
cpg	235.02	J/mol×K	507.83	Joback Method
cpg	221.85	J/mol×K	473.71	Joback Method
cpg	208.06	J/mol×K	439.58	Joback Method

cpg	193.64	J/mol×K	405.46	Joback Method
dvisc	0.0052904	Pa×s	213.66	Joback Method
dvisc	0.0003666	Pa×s	405.46	Joback Method
dvisc	0.0004728	Pa×s	373.49	Joback Method
dvisc	0.0006396	Pa×s	341.53	Joback Method
dvisc	0.0009210	Pa×s	309.56	Joback Method
dvisc	0.0014422	Pa×s	277.59	Joback Method
dvisc	0.0025382	Pa×s	245.63	Joback Method
hvapt	39.10	kJ/mol	380.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1121206&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/11-098-1/trans-4-5-Dimethyl-1-3-dioxane.pdf>

Generated by Cheméo on 2025-12-18 20:31:59.700612858 +0000 UTC m=+5838117.230653527.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.