

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+
InchiKey:	OCBJIXQOIASAQK-OLQVQODUSA-N
Formula:	C6H12O2
SMILES:	CC1CC(C)OCO1
Mol. weight [g/mol]:	116.16
CAS:	3390-18-9

Physical Properties

Property code	Value	Unit	Source
chl	-3601.30 ± 2.40	kJ/mol	NIST Webbook
gf	-155.86	kJ/mol	Joback Method
hf	-397.19	kJ/mol	Joback Method
hfl	-474.80 ± 2.40	kJ/mol	NIST Webbook
hfus	20.16	kJ/mol	Joback Method
hvap	38.09	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	1.158		Crippen Method
mcvol	96.280	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
tb	388.15 ± 1.50	K	NIST Webbook
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	193.64	J/mol×K	405.46	Joback Method
cpg	208.06	J/mol×K	439.58	Joback Method
cpg	221.85	J/mol×K	473.71	Joback Method
cpg	235.02	J/mol×K	507.83	Joback Method
cpg	247.58	J/mol×K	541.95	Joback Method
cpg	259.54	J/mol×K	576.08	Joback Method
cpg	270.89	J/mol×K	610.20	Joback Method

dvisc	0.0052904	Pa×s	213.66	Joback Method
dvisc	0.0025382	Pa×s	245.63	Joback Method
dvisc	0.0014422	Pa×s	277.59	Joback Method
dvisc	0.0009210	Pa×s	309.56	Joback Method
dvisc	0.0006396	Pa×s	341.53	Joback Method
dvisc	0.0004728	Pa×s	373.49	Joback Method
dvisc	0.0003666	Pa×s	405.46	Joback Method

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=C3390189&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
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

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