

1,4-Dioxane, 2,3-dichloro-

Other names:	p-Dioxane, 2,3-dichloro- 2,3-Dichloro-p-dioxane 2,3-Dichloro-1,4-dioxane
Inchi:	InChI=1S/C4H6Cl2O2/c5-3-4(6)8-2-1-7-3/h3-4H,1-2H2
InchiKey:	ZOZUXFQYIYUIND-UHFFFAOYSA-N
Formula:	C4H6Cl2O2
SMILES:	C1C1OCCOC1Cl
Mol. weight [g/mol]:	157.00
CAS:	95-59-0

Physical Properties

Property code	Value	Unit	Source
gf	-196.56	kJ/mol	Joback Method
hf	-387.39	kJ/mol	Joback Method
hfus	23.37	kJ/mol	Joback Method
hvap	42.41	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	1.163		Crippen Method
mcvol	92.580	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
tb	434.56	K	Joback Method
tc	659.62	K	Joback Method
tf	250.96	K	Joback Method
vc	0.332	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.26	J/mol×K	434.56	Joback Method
cpg	217.46	J/mol×K	622.11	Joback Method
cpg	208.96	J/mol×K	584.60	Joback Method
cpg	199.90	J/mol×K	547.09	Joback Method
cpg	190.26	J/mol×K	509.58	Joback Method
cpg	180.05	J/mol×K	472.07	Joback Method

cpg	225.41	J/mol×K	659.62	Joback Method
dvisc	0.0004789	Pa×s	434.56	Joback Method
dvisc	0.0006070	Pa×s	403.96	Joback Method
dvisc	0.0007999	Pa×s	373.36	Joback Method
dvisc	0.0011073	Pa×s	342.76	Joback Method
dvisc	0.0016337	Pa×s	312.16	Joback Method
dvisc	0.0026231	Pa×s	281.56	Joback Method
dvisc	0.0047272	Pa×s	250.96	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=C95590&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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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