1,3-Dioxane, 2-methyl-

Other names:	m-Dioxane, 2-methyl-
	2-Methyl-m-dioxane
	2-Methyl-1,3-dioxane
	2-Methyl-1,3-dioxacyclohexane
Inchi:	InChI=1S/C5H10O2/c1-5-6-3-2-4-7-5/h5H,2-4H2,1H3
InchiKey:	HDGHQFQMWUTHKL-UHFFFAOYSA-N
Formula:	C5H10O2
SMILES:	CC1OCCCO1
Mol. weight [g/mol]:	102.13
CAS:	626-68-6

Physical Properties

Property code	Value	Unit	Source
chl	-2960.30 ± 2.60	kJ/mol	NIST Webbook
chl	-2959.10 ± 1.00	kJ/mol	NIST Webbook
gf	-156.57	kJ/mol	Joback Method
hf	-397.50 ± 2.80	kJ/mol	NIST Webbook
hf	-399.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-436.50 ± 2.60	kJ/mol	NIST Webbook
hfus	16.50	kJ/mol	Joback Method
hvap	39.00 ± 1.00	kJ/mol	NIST Webbook
ie	10.03	eV	NIST Webbook
log10ws	-0.59		Crippen Method
logp	0.769		Crippen Method
mcvol	82.190	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
ripol	1044.00		NIST Webbook
tb	377.65 ± 1.50	K	NIST Webbook
tc	594.41	K	Joback Method
tf	206.63	K	Joback Method
vc	0.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.92	J/mol×K	387.25	Joback Method
cpg	213.09	J/mol×K	559.89	Joback Method
cpg	202.61	J/mol×K	525.36	Joback Method
cpg	191.56	J/mol×K	490.83	Joback Method
cpg	179.94	J/mol×K	456.30	Joback Method
cpg	167.72	J/mol×K	421.78	Joback Method
cpg	223.02	J/mol×K	594.41	Joback Method
dvisc	0.0003961	Pa×s	387.25	Joback Method
dvisc	0.0005325	Pa×s	357.15	Joback Method
dvisc	0.0007559	Pa×s	327.04	Joback Method
dvisc	0.0011521	Pa×s	296.94	Joback Method
dvisc	0.0019309	Pa×s	266.84	Joback Method
dvisc	0.0036904	Pa×s	236.73	Joback Method
dvisc	0.0085183	Pa×s	206.63	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C626686&Units=SI

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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume