

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	-2959.10 ± 1.00	kJ/mol	NIST Webbook
chl	-2960.30 ± 2.60	kJ/mol	NIST Webbook
gf	-156.57	kJ/mol	Joback Method
hf	-399.00 ± 3.00	kJ/mol	NIST Webbook
hf	-397.50 ± 2.80	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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