1,3-Dioxane, 2,4-dimethyl-

Other names:	m-Dioxane, 2,4-dimethyl-
	2,4-Dimethyl-m-dioxane
	2,4-Dimethyl-1,3-dioxane
Inchi:	InChI=1S/C6H12O2/c1-5-3-4-7-6(2)8-5/h5-6H,3-4H2,1-2H3
InchiKey:	VREPYGYMOSZTKJ-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CC1CCOC(C)O1
Mol. weight [g/mol]:	116.16
CAS:	766-20-1

Physical Properties

Property code	Value	Unit	Source
gf	-155.86	kJ/mol	Joback Method
hf	-397.19	kJ/mol	Joback Method
hfus	20.16	kJ/mol	Joback Method
hvap	44.90 ± 0.60	kJ/mol	NIST Webbook
ie	9.90	eV	NIST Webbook
log10ws	-1.12		Crippen Method
logp	1.158		Crippen Method
mcvol	96.280	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	786.00		NIST Webbook
rinpol	786.00		NIST Webbook
ripol	1072.00		NIST Webbook
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	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: 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=C766201&Units=SI

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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume