1,3-Dioxane, 4,5-dimethyl-

Other names: m-Dioxane, 4,5-dimethyl-
5,6-Dimethyl-1,3-dioxane
4,5-Dimethyl-1,3-dioxane
Inchi: InChI=1S/C6H12O2/c1-5-3-7-4-8-6(5)2/h5-6H,3-4H2,1-2H3
InchiKey: YMXZGCMNTIZHDC-UHFFFAOYSA-N
Formula: C6H12O2
SMILES: CC1COCOC1C
Mol. weight [g/mol]: 116.16
CAS: 1779-22-2

Physical Properties

Property code	Value	Unit	Source
chl	-3624.40 ± 2.00	kJ/mol	NIST Webbook
gf	-155.86	kJ/mol	Joback Method
hf	-397.19	kJ/mol	Joback Method
hfl	-451.70 ± 2.00	kJ/mol	NIST Webbook
hfus	20.16	kJ/mol	Joback Method
hvap	38.09	kJ/mol	Joback Method
log10ws	-0.77		Crippen Method
logp	1.015		Crippen Method
mcvol	96.280	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
tb	404.65 ± 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

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=C1779222&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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