2-Hydroxymethyl-1,3-dioxane

Inchi: InChI=1S/C5H10O3/c6-4-5-7-2-1-3-8-5/h5-6H,1-4H2
InchiKey: IEBHUKYDOBADIB-UHFFFAOYSA-N
Formula: C5H10O3
SMILES: OCC1OCCCO1
Mol. weight [g/mol]: 118.13
CAS: 39239-93-5

Physical Properties

Property code	Value	Unit	Source
chl	-2773.60 ± 4.90	kJ/mol	NIST Webbook
gf	-293.39	kJ/mol	Joback Method
hf	-554.00 ± 12.00	kJ/mol	NIST Webbook
hfl	-623.00 ± 10.00	kJ/mol	NIST Webbook
hfus	20.59	kJ/mol	Joback Method
hvap	69.00 ± 2.00	kJ/mol	NIST Webbook
hvap	69.00	kJ/mol	NIST Webbook
log10ws	0.14		Crippen Method
logp	-0.258		Crippen Method
mcvol	88.060	ml/mol	McGowan Method
pc	4966.33	kPa	Joback Method
tb	479.43	K	Joback Method
tc	675.81	K	Joback Method
tf	267.45	K	Joback Method
vc	0.309	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.46	J/mol×K	479.43	Joback Method
cpg	253.26	J/mol×K	643.08	Joback Method
cpg	244.35	J/mol×K	610.35	Joback Method
cpg	234.93	J/mol×K	577.62	Joback Method
cpg	224.98	J/mol×K	544.89	Joback Method
cpg	214.49	J/mol×K	512.16	Joback Method

cpg	261.67	J/mol×K	675.81	Joback Method
dvisc	0.0002452	Pa×s	479.43	Joback Method
dvisc	0.0004087	Pa×s	444.10	Joback Method
dvisc	0.0007442	Pa×s	408.77	Joback Method
dvisc	0.0015175	Pa×s	373.44	Joback Method
dvisc	0.0035916	Pa×s	338.11	Joback Method
dvisc	0.0103930	Pa×s	302.78	Joback Method
dvisc	0.0398209	Pa×s	267.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39239935&Units=SI
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

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