1,3-Propanediol, 2,2-dimethyl-, diformate

Inchi: InChI=1S/C7H12O4/c1-7(2,3-10-5-8)4-11-6-9/h5-6H,3-4H2,1-2H3
InchiKey: KDZSXEAXMYXVCU-UHFFFAOYSA-N
Formula: C7H12O4
SMILES: CC(C)(COC=O)COC=O
Mol. weight [g/mol]: 160.17
CAS: 5451-58-1

Physical Properties

Property code	Value	Unit	Source
gf	-398.14	kJ/mol	Joback Method
hf	-632.16	kJ/mol	Joback Method
hfus	13.43	kJ/mol	Joback Method
hvap	48.14	kJ/mol	Joback Method
log10ws	-0.24		Crippen Method
logp	0.359		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
tb	498.49	K	Joback Method
tc	686.09	K	Joback Method
tf	299.53	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.52	J/mol×K	498.49	Joback Method
cpg	295.16	J/mol×K	529.76	Joback Method
cpg	305.31	J/mol×K	561.02	Joback Method
cpg	315.00	J/mol×K	592.29	Joback Method
cpg	324.21	J/mol×K	623.56	Joback Method
cpg	332.96	J/mol×K	654.82	Joback Method
cpg	341.26	J/mol×K	686.09	Joback Method
dvisc	0.0033082	Pa×s	299.53	Joback Method
dvisc	0.0017937	Pa×s	332.69	Joback Method

dvisc	0.0010867	Pa×s	365.85	Joback Method
dvisc	0.0007155	Pa×s	399.01	Joback Method
dvisc	0.0005023	Pa×s	432.17	Joback Method
dvisc	0.0003709	Pa×s	465.33	Joback Method
dvisc	0.0002851	Pa×s	498.49	Joback Method

Sources

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=C5451581&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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