Glycerol, triformate

Other names: 1,2,3-Propanetriol, 1,2,3-triformate
Inchi: InChI=1S/C6H8O6/c7-3-10-1-6(12-5-9)2-11-4-8/h3-6H,1-2H2
InchiKey: UFTFJSFQGQCHQW-UHFFFAOYSA-N
Formula: C6H8O6
SMILES: O=COCC(COC=O)OC=O
Mol. weight [g/mol]: 176.12
CAS: 32765-69-8

Physical Properties

Property code	Value	Unit	Source
gf	-616.36	kJ/mol	Joback Method
hf	-825.85	kJ/mol	Joback Method
hfus	18.20	kJ/mol	Joback Method
hvap	55.95	kJ/mol	Joback Method
log10ws	0.97		Crippen Method
logp	-1.126		Crippen Method
mcvol	117.720	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	1120.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1118.00		NIST Webbook
tb	549.48	K	Joback Method
tc	735.58	K	Joback Method
tf	335.07	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.91	J/mol×K	549.48	Joback Method
cpg	312.51	J/mol×K	704.56	Joback Method
cpg	305.62	J/mol×K	673.55	Joback Method

cpg	298.40	J/mol×K	642.53	Joback Method
cpg	290.86	J/mol×K	611.51	Joback Method
cpg	283.02	J/mol×K	580.50	Joback Method
cpg	319.03	J/mol×K	735.58	Joback Method
dvisc	0.0002863	Pa×s	549.48	Joback Method
dvisc	0.0003622	Pa×s	513.75	Joback Method
dvisc	0.0004745	Pa×s	478.01	Joback Method
dvisc	0.0006496	Pa×s	442.27	Joback Method
dvisc	0.0009396	Pa×s	406.54	Joback Method
dvisc	0.0014594	Pa×s	370.81	Joback Method
dvisc	0.0024898	Pa×s	335.07	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C32765698&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

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume