Citric acid, trimethyl ester

Other names:	1,2,3-Propanetricarboxylic acid, 2-hydroxy-, trimethyl ester
	Trimethyl citrate
	3-Hydroxy-3-methoxycarbonylpentanedioic acid, dimethyl ester
Inchi:	InChI=1S/C9H14O7/c1-14-6(10)4-9(13,8(12)16-3)5-7(11)15-2/h13H,4-5H2,1-3H3
InchiKey:	HDDLVZWGOPWKFW-UHFFFAOYSA-N
Formula:	C9H14O7
SMILES:	COC(=O)CC(O)(CC(=O)OC)C(=O)OC
Mol. weight [g/mol]:	234.20
CAS:	1587-20-8

Physical Properties

Property code	Value	Unit	Source
gf	-810.84	kJ/mol	Joback Method
hf	-1124.47	kJ/mol	Joback Method
hfus	24.10	kJ/mol	Joback Method
hvap	78.48	kJ/mol	Joback Method
log10ws	0.45		Crippen Method
logp	-0.983		Crippen Method
mcvol	165.860	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	1442.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1442.00		NIST Webbook
tb	723.14	K	Joback Method
tc	912.95	K	Joback Method
tf	470.91	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.78	J/mol×K	723.14	Joback Method
cpg	471.58	J/mol×K	754.77	Joback Method
cpg	480.77	J/mol×K	786.41	Joback Method
cpg	489.33	J/mol×K	818.04	Joback Method
cpg	497.27	J/mol×K	849.68	Joback Method
cpg	504.58	J/mol×K	881.31	Joback Method
cpg	511.25	J/mol×K	912.95	Joback Method
dvisc	0.0006814	Pa×s	470.91	Joback Method
dvisc	0.0003268	Pa×s	512.95	Joback Method
dvisc	0.0001751	Pa×s	554.99	Joback Method
dvisc	0.0001025	Pa×s	597.02	Joback Method
dvisc	0.0000644	Pa×s	639.06	Joback Method
dvisc	0.0000428	Pa×s	681.10	Joback Method
dvisc	0.0000299	Pa×s	723.14	Joback Method
hvapt	617.40	kJ/mol	469.50	NIST Webbook

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=C1587208&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt: Enthalpy of vaporization at a given temperature

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