Tricarballylic acid

Other names:	1,2,3-Propanetricarboxylic acid
	«beta»-Carboxyglutaric acid
	Carballylic acid
	Propane 1,2,3-tricarboxylic acid
	Tricarballylate
Inchi:	InChI=1S/C6H8O6/c7-4(8)1-3(6(11)12)2-5(9)10/h3H,1-2H2,(H,7,8)(H,9,10)(H,11,12)
InchiKey:	KQTIIICEAUMSDG-UHFFFAOYSA-N
Formula:	C6H8O6
SMILES:	O=C(O)CC(CC(=O)O)C(=O)O
Mol. weight [g/mol]:	176.12
CAS:	99-14-9

Physical Properties

Property code	Value	Unit	Source
gf	-800.02	kJ/mol	Joback Method
hf	-966.88	kJ/mol	Joback Method
hfus	24.83	kJ/mol	Joback Method
hvap	98.84	kJ/mol	Joback Method
log10ws	0.61		Crippen Method
logp	-0.363		Crippen Method
mcvol	117.720	ml/mol	McGowan Method
pc	5730.52	kPa	Joback Method
tb	774.39	K	Joback Method
tc	958.00	K	Joback Method
tf	474.63	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.91	J/mol×K	774.39	Joback Method
cpg	344.25	J/mol×K	927.40	Joback Method
cpg	340.25	J/mol×K	896.80	Joback Method
cpg	335.93	J/mol×K	866.19	Joback Method

cpg	331.27	J/mol×K	835.59	Joback Method
cpg	326.27	J/mol×K	804.99	Joback Method
cpg	347.93	J/mol×K	958.00	Joback Method
dvisc	0.0000032	Pa×s	774.39	Joback Method
dvisc	0.0000058	Pa×s	724.43	Joback Method
dvisc	0.0000116	Pa×s	674.47	Joback Method
dvisc	0.0000260	Pa×s	624.51	Joback Method
dvisc	0.0000671	Pa×s	574.55	Joback Method
dvisc	0.0002075	Pa×s	524.59	Joback Method
dvisc	0.0008139	Pa×s	474.63	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=C99149&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
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