

Methyltartronic acid

Inchi:	InChI=1S/C4H6O5/c1-4(9,2(5)6)3(7)8/h9H,1H3,(H,5,6)(H,7,8)
InchiKey:	LNRVTEQEGXVMEF-UHFFFAOYSA-N
Formula:	C4H6O5
SMILES:	CC(O)(C(=O)O)C(=O)O
Mol. weight [g/mol]:	134.09
CAS:	595-98-2

Physical Properties

Property code	Value	Unit	Source
gf	-682.66	kJ/mol	Joback Method
hf	-816.49	kJ/mol	Joback Method
hfus	14.16	kJ/mol	Joback Method
hvap	86.73	kJ/mol	Joback Method
log10ws	0.93		Crippen Method
logp	-1.093		Crippen Method
mcvol	87.970	ml/mol	McGowan Method
pc	7169.69	kPa	Joback Method
tb	671.97	K	Joback Method
tc	850.48	K	Joback Method
tf	419.58	K	Joback Method
vc	0.318	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.65	J/mol×K	671.97	Joback Method
cpg	230.08	J/mol×K	701.72	Joback Method
cpg	234.21	J/mol×K	731.47	Joback Method
cpg	238.06	J/mol×K	761.23	Joback Method
cpg	241.65	J/mol×K	790.98	Joback Method
cpg	245.01	J/mol×K	820.73	Joback Method
cpg	248.14	J/mol×K	850.48	Joback Method
dvisc	0.0027201	Pa×s	419.58	Joback Method
dvisc	0.0006518	Pa×s	461.65	Joback Method

dvisc	0.0001983	Pa×s	503.71	Joback Method
dvisc	0.0000725	Pa×s	545.78	Joback Method
dvisc	0.0000306	Pa×s	587.84	Joback Method
dvisc	0.0000145	Pa×s	629.90	Joback Method
dvisc	0.0000075	Pa×s	671.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C595982&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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