

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/molxK	671.97	Joback Method
cpg	230.08	J/molxK	701.72	Joback Method
cpg	234.21	J/molxK	731.47	Joback Method
cpg	238.06	J/molxK	761.23	Joback Method
cpg	241.65	J/molxK	790.98	Joback Method
cpg	245.01	J/molxK	820.73	Joback Method
cpg	248.14	J/molxK	850.48	Joback Method
dvisc	0.0027201	Paxs	419.58	Joback Method
dvisc	0.0006518	Paxs	461.65	Joback Method

dvisc	0.0001983	Paxs	503.71	Joback Method
dvisc	0.0000725	Paxs	545.78	Joback Method
dvisc	0.0000306	Paxs	587.84	Joback Method
dvisc	0.0000145	Paxs	629.90	Joback Method
dvisc	0.0000075	Paxs	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/ci9903071
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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