(E)-1-Propene-1,2,3-tricarboxylic acid

Other names: 1-Propene-1,2,3-tricarboxylic acid, trans
1-Propene-1,trans-2,3-tricarboxylic acid
1-propene-1,2,3-tricarboxylic acid, (E)-
Aconitic acid, trans
E-1-propene-1,2,3-tricarboxylic acid, tributyl ester
trans-1,2,3-propenetricarboxylic acid
trans-1-propene-1,2,3-tricarboxylic acid
trans-Aconitate
trans-achilleaic acid
trans-achilleic acid
trans-aconitic acid
trans-citridinic acid
trans-equisetic acid
trans-pyrocitric acid

Inchi: InChI=1S/C6H6O6/c7-4(8)1-3(6(11)12)2-5(9)10/h1H,2H2,(H,7,8)(H,9,10)(H,11,12)/b3-1+

InchiKey: GTZCVFVGUGFEME-HNQUOIGGSA-N

Formula: C6H6O6

SMILES: O=C(O)C=C(CC(=O)O)C(=O)O

Mol. weight [g/mol]: 174.11

CAS: 4023-65-8

Physical Properties

Property code	Value	Unit	Source
chs	-1985.80 ± 2.50	kJ/mol	NIST Webbook
gf	-725.91	kJ/mol	Joback Method
hf	-854.17	kJ/mol	Joback Method
hfs	-1233.00 ± 3.00	kJ/mol	NIST Webbook
hfus	27.25	kJ/mol	Joback Method
hvap	99.26	kJ/mol	Joback Method
log10ws	0.51		Crippen Method
logp	-0.443		Crippen Method
mcvol	113.420	ml/mol	McGowan Method
pc	6180.53	kPa	Joback Method
tb	778.87	K	Joback Method
tc	966.03	K	Joback Method
tf	455.75 ± 0.80	K	NIST Webbook
tf	456.45 ± 0.60	K	NIST Webbook

vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.62	J/mol×K	778.87	Joback Method
cpg	298.29	J/mol×K	810.06	Joback Method
cpg	302.67	J/mol×K	841.26	Joback Method
cpg	306.77	J/mol×K	872.45	Joback Method
cpg	310.61	J/mol×K	903.64	Joback Method
cpg	314.22	J/mol×K	934.84	Joback Method
cpg	317.62	J/mol×K	966.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4023658&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Effect of Diluents on Extraction Equilibrium of trans-Aconitic Acid:	https://www.doi.org/10.1021/acs.jced.9b00059
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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