Citraconic acid

Other names: 2-methyl-2-butenedioic acid
Inchi: InChI=1S/C5H6O4/c1-3(5(8)9)2-4(6)7/h2H,1H3,(H,6,7)(H,8,9)/b3-2-
InchiKey: HNEGQIOMVPPMNR-IHWYPQMZSA-N
Formula: C5H6O4
SMILES: CC(=CC(=O)O)C(=O)O
Mol. weight [g/mol]: 130.10
CAS: 7407-59-2

Physical Properties

Property code	Value	Unit	Source
gf	-468.59	kJ/mol	Joback Method
hf	-568.72	kJ/mol	Joback Method
hfus	18.97	kJ/mol	Joback Method
hvap	73.61	kJ/mol	Joback Method
log10ws	0.03		Crippen Method
logp	0.102		Crippen Method
mcvol	91.890	ml/mol	McGowan Method
pc	5644.74	kPa	Joback Method
tb	609.94	K	Joback Method
tc	793.59	K	Joback Method
tf	348.57	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.67	J/mol×K	609.94	Joback Method
cpg	216.17	J/mol×K	640.55	Joback Method
cpg	221.35	J/mol×K	671.16	Joback Method
cpg	226.24	J/mol×K	701.77	Joback Method
cpg	230.85	J/mol×K	732.37	Joback Method
cpg	235.19	J/mol×K	762.98	Joback Method
cpg	239.29	J/mol×K	793.59	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7407592&Units=SI

Legend

cpg:	Ideal gas heat capacity
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