Butanedioic acid, methylene-

Other names:	2-Propene-1,2-dicarboxylic acid
	3-carboxy-3-butenoic acid
	Butanedioic acid, 2-methylene-
	Itaconic acid
	Methylenebutanedioic acid
	Methylenesuccinic acid
	Propylenedicarboxylic acid
	Succinic acid, methylene-
	methylene-1,4-butanedioic acid
Inchi:	InChI=1S/C5H6O4/c1-3(5(8)9)2-4(6)7/h1-2H2,(H,6,7)(H,8,9)
InchiKey:	LVHBHZANLOWSRM-UHFFFAOYSA-N
Formula:	C5H6O4
SMILES:	C=C(CC(=O)O)C(=O)O
Mol. weight [g/mol]:	130.10
CAS:	97-65-4

Physical Properties

Property code	Value	Unit	Source
chs	-1983.90 ± 0.50	kJ/mol	NIST Webbook
gf	-460.97	kJ/mol	Joback Method
hf	-560.51	kJ/mol	Joback Method
hfs	-841.11 ± 0.59	kJ/mol	NIST Webbook
hfus	17.49	kJ/mol	Joback Method
hvap	72.98	kJ/mol	Joback Method
log10ws	-0.22		Aqueous Solubility Prediction Method
logp	0.102		Crippen Method
mcvol	91.890	ml/mol	McGowan Method
pc	5560.87	kPa	Joback Method
tb	602.46	K	Joback Method
tc	782.44	K	Joback Method
tf	438.25 ± 1.00	K	NIST Webbook
tf	440.15	K	Solubility of itaconic acid in different organic solvents: Experimental measurement and thermodynamic modeling
tf	439.00 ± 0.70	K	NIST Webbook

vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.91	J/mol×K	602.46	Joback Method
cpg	217.40	J/mol×K	632.46	Joback Method
cpg	222.59	J/mol×K	662.45	Joback Method
cpg	227.50	J/mol×K	692.45	Joback Method
cpg	232.13	J/mol×K	722.45	Joback Method
cpg	236.50	J/mol×K	752.44	Joback Method
cpg	240.61	J/mol×K	782.44	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.68658e+01
Coeff. B	-9.28405e+03
Coeff. C	-1.23842e+02
Temperature range (K), min.	473.15
Temperature range (K), max.	554.57

Sources

Solubility of itaconic acid in different organic solvents: Experimental measurement and thermodynamic modeling:	https://www.doi.org/10.1016/j.fluid.2011.09.027
Volumetric properties of itaconic acid aqueous solutions:	https://www.doi.org/10.1016/j.jct.2011.09.014
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97654&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume