4-Methyl itaconate

Other names: Butanedioic acid, methylene-, 4-methyl ester
4-methyl hydrogen 2-methylenesuccinate
Inchi: InChI=1S/C6H8O4/c1-4(6(8)9)3-5(7)10-2/h1,3H2,2H3,(H,8,9)
InchiKey: OIYTYGOUZOARSH-UHFFFAOYSA-N
Formula: C6H8O4
SMILES: C=C(CC(=O)OC)C(=O)O
Mol. weight [g/mol]: 144.13
CAS: 7338-27-4

Physical Properties

Property code	Value	Unit	Source
gf	-420.73	kJ/mol	Joback Method
hf	-561.14	kJ/mol	Joback Method
hfus	17.18	kJ/mol	Joback Method
hvap	60.94	kJ/mol	Joback Method
log10ws	-0.15		Crippen Method
logp	0.190		Crippen Method
mcvol	105.980	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
tb	555.58	K	Joback Method
tc	741.35	K	Joback Method
tf	324.57	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.60	J/mol×K	555.58	Joback Method
cpg	246.18	J/mol×K	586.54	Joback Method
cpg	253.42	J/mol×K	617.50	Joback Method
cpg	260.31	J/mol×K	648.47	Joback Method
cpg	266.86	J/mol×K	679.43	Joback Method
cpg	273.07	J/mol×K	710.39	Joback Method
cpg	278.94	J/mol×K	741.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7338274&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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