2-Isopropylidenebutanedioic acid

Other names: Isopropylidene-succinic acid
Inchi: InChI=1S/C7H10O4/c1-4(2)5(7(10)11)3-6(8)9/h3H2,1-2H3,(H,8,9)(H,10,11)
InchiKey: GYXGAEAOIFNGAE-UHFFFAOYSA-N
Formula: C7H10O4
SMILES: CC(C)=C(CC(=O)O)C(=O)O
Mol. weight [g/mol]: 158.15
CAS: 584-27-0

Physical Properties

Property code	Value	Unit	Source
gf	-460.30	kJ/mol	Joback Method
hf	-619.79	kJ/mol	Joback Method
hfus	22.84	kJ/mol	Joback Method
hvap	78.14	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	0.882		Crippen Method
mcvol	120.070	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	655.58	K	Joback Method
tc	838.83	K	Joback Method
tf	357.15	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.22	J/mol×K	655.58	Joback Method
cpg	308.54	J/mol×K	686.12	Joback Method
cpg	315.48	J/mol×K	716.66	Joback Method
cpg	322.03	J/mol×K	747.21	Joback Method
cpg	328.24	J/mol×K	777.75	Joback Method
cpg	334.11	J/mol×K	808.29	Joback Method
cpg	339.67	J/mol×K	838.83	Joback Method

Sources

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=C584270&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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