(-)-2,3-Dimethylbutanedioic acid

Inchi: InChI=1S/C6H10O4/c1-3(5(7)8)4(2)6(9)10/h3-4H,1-2H3,(H,7,8)(H,9,10)/t3-,4-/m0/s1
InchiKey: KLZYRCVPDWTZLH-IMJSIDKUSA-N
Formula: C6H10O4
SMILES: CC(C(=O)O)C(C)C(=O)O
Mol. weight [g/mol]: 146.14
CAS: 57694-62-9

Physical Properties

Property code	Value	Unit	Source
chs	-2807.70 ± 1.40	kJ/mol	NIST Webbook
gf	-536.72	kJ/mol	Joback Method
hf	-707.35	kJ/mol	Joback Method
hfus	15.62	kJ/mol	Joback Method
hvap	75.02	kJ/mol	Joback Method
log10ws	-0.05		Crippen Method
logp	0.428		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	4640.32	kPa	Joback Method
tb	627.90	K	Joback Method
tc	807.19	K	Joback Method
tf	348.88	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.61	J/mol×K	627.90	Joback Method
cpg	285.95	J/mol×K	657.78	Joback Method
cpg	292.90	J/mol×K	687.66	Joback Method
cpg	299.49	J/mol×K	717.55	Joback Method
cpg	305.72	J/mol×K	747.43	Joback Method
cpg	311.60	J/mol×K	777.31	Joback Method
cpg	317.14	J/mol×K	807.19	Joback Method
dvisc	0.0165669	Pa×s	348.88	Joback Method

dvisc	0.0031943	Pa×s	395.38	Joback Method
dvisc	0.0008709	Pa×s	441.89	Joback Method
dvisc	0.0003041	Pa×s	488.39	Joback Method
dvisc	0.0001275	Pa×s	534.89	Joback Method
dvisc	0.0000614	Pa×s	581.40	Joback Method
dvisc	0.0000330	Pa×s	627.90	Joback Method

Sources

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=C57694629&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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