

Butanedioic acid, hydroxy-, (S)-

Other names:	Malic acid, L- (-)-Hydroxysuccinic acid (-)-Malic acid (S)-Malic acid Apple acid L-(-)-Malic acid L-Malic acid S-(-)-Malic acid (S)-Hydroxybutanedioic acid Malic acid-, (L-form)- (2S)-2-Hydroxybutanedioic acid Butanedioic acid, 2-hydroxy-, (2S)- Butanedioic acid, hydroxy-, (2S)- NSC 9232 S-2-Hydroxybutanedioic acid
Inchi:	InChI=1S/C4H6O5/c5-2(4(8)9)1-3(6)7/h2,5H,1H2,(H,6,7)(H,8,9)/t2-/m1/s1
InchiKey:	BJEPYKJPYRNKOW-UWTATZPHSA-N
Formula:	C4H6O5
SMILES:	O=C(O)CC(O)C(=O)O
Mol. weight [g/mol]:	134.09
CAS:	97-67-6

Physical Properties

Property code	Value	Unit	Source
chs	-1328.00 ± 4.20	kJ/mol	NIST Webbook
gf	-687.94	kJ/mol	Joback Method
hf	-813.02	kJ/mol	Joback Method
hfs	-1103.70 ± 4.20	kJ/mol	NIST Webbook
hfus	18.05	kJ/mol	Joback Method
hvap	87.64	kJ/mol	Joback Method
log10ws	0.93		Crippen Method
logp	-1.093		Crippen Method
mcvol	87.970	ml/mol	McGowan Method
pc	7037.97	kPa	Joback Method
tb	674.76	K	Joback Method
tc	849.14	K	Joback Method
tf	372.70 ± 0.70	K	NIST Webbook

vc	0.323	m ³ /kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.47	J/mol×K	674.76	Joback Method
cpg	227.04	J/mol×K	703.82	Joback Method
cpg	231.36	J/mol×K	732.89	Joback Method
cpg	235.42	J/mol×K	761.95	Joback Method
cpg	239.25	J/mol×K	791.02	Joback Method
cpg	242.84	J/mol×K	820.08	Joback Method
cpg	246.21	J/mol×K	849.14	Joback Method
dvisc	0.0048344	Pa×s	402.16	Joback Method
dvisc	0.0009670	Pa×s	447.59	Joback Method
dvisc	0.0002602	Pa×s	493.03	Joback Method
dvisc	0.0000874	Pa×s	538.46	Joback Method
dvisc	0.0000348	Pa×s	583.89	Joback Method
dvisc	0.0000158	Pa×s	629.33	Joback Method
dvisc	0.0000080	Pa×s	674.76	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=C97676&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

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

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