

Butanoic acid, 4-hydroxy-

Other names:	GHB «gamma»-Hydroxybutyric acid decomposition product 4-Hydroxybutyric acid
Inchi:	InChI=1S/C4H8O3/c5-3-1-2-4(6)7/h5H,1-3H2,(H,6,7)
InchiKey:	SJZRECIVHVDYJC-UHFFFAOYSA-N
Formula:	C4H8O3
SMILES:	O=C(O)CCCO
Mol. weight [g/mol]:	104.10
CAS:	591-81-1

Physical Properties

Property code	Value	Unit	Source
gf	-419.76	kJ/mol	Joback Method
hf	-542.93	kJ/mol	Joback Method
hfl	-710.00 ± 3.00	kJ/mol	NIST Webbook
hfus	15.89	kJ/mol	Joback Method
hvap	64.60	kJ/mol	Joback Method
log10ws	0.14		Crippen Method
logp	-0.157		Crippen Method
mcvol	80.530	ml/mol	McGowan Method
pc	5446.55	kPa	Joback Method
rinpol	933.00		NIST Webbook
rinpol	933.00		NIST Webbook
tb	529.15	K	Joback Method
tc	696.80	K	Joback Method
tf	306.41	K	Joback Method
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.35	J/mol×K	529.15	Joback Method
cpg	209.17	J/mol×K	668.86	Joback Method
cpg	204.28	J/mol×K	640.92	Joback Method

cpg	199.15	J/mol×K	612.98	Joback Method
cpg	193.79	J/mol×K	585.03	Joback Method
cpg	188.20	J/mol×K	557.09	Joback Method
cpg	213.85	J/mol×K	696.80	Joback Method
dvisc	0.0000866	Pa×s	529.15	Joback Method
dvisc	0.0001615	Pa×s	492.03	Joback Method
dvisc	0.0003335	Pa×s	454.90	Joback Method
dvisc	0.0007835	Pa×s	417.78	Joback Method
dvisc	0.0021744	Pa×s	380.66	Joback Method
dvisc	0.0075235	Pa×s	343.53	Joback Method
dvisc	0.0351663	Pa×s	306.41	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=C591811&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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