

Hexanoic acid, 6-hydroxy-

Other names:	6-Hydroxycaproic acid 6-Hydroxyhexanoic acid
Inchi:	InChI=1S/C6H12O3/c7-5-3-1-2-4-6(8)9/h7H,1-5H2,(H,8,9)
InchiKey:	IWHLYPDWHPVAA-UHFFFAOYSA-N
Formula:	C6H12O3
SMILES:	O=C(O)CCCCO
Mol. weight [g/mol]:	132.16
CAS:	1191-25-9

Physical Properties

Property code	Value	Unit	Source
gf	-402.92	kJ/mol	Joback Method
hf	-584.21	kJ/mol	Joback Method
hfs	-786.00 ± 3.00	kJ/mol	NIST Webbook
hfus	21.07	kJ/mol	Joback Method
hvap	69.05	kJ/mol	Joback Method
log10ws	-0.70		Crippen Method
logp	0.624		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	4178.49	kPa	Joback Method
tb	574.91	K	Joback Method
tc	740.78	K	Joback Method
tf	328.95	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.77	J/molxK	574.91	Joback Method
cpg	275.55	J/molxK	602.56	Joback Method
cpg	283.00	J/molxK	630.20	Joback Method
cpg	290.13	J/molxK	657.85	Joback Method
cpg	296.95	J/molxK	685.49	Joback Method
cpg	303.46	J/molxK	713.14	Joback Method

cpg	309.68	J/mol×K	740.78	Joback Method
dvisc	0.0199932	Paxs	328.95	Joback Method
dvisc	0.0043019	Paxs	369.94	Joback Method
dvisc	0.0012576	Paxs	410.94	Joback Method
dvisc	0.0004596	Paxs	451.93	Joback Method
dvisc	0.0001985	Paxs	492.92	Joback Method
dvisc	0.0000976	Paxs	533.92	Joback Method
dvisc	0.0000531	Paxs	574.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1191259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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