

methyl 4-hydroxyhexanoate

Inchi:	InChI=1S/C7H14O3/c1-3-6(8)4-5-7(9)10-2/h6,8H,3-5H2,1-2H3
InchiKey:	GAHDIGHBYWYMPW-UHFFFAOYSA-N
Formula:	C7H14O3
SMILES:	CCC(O)CCC(=O)OC
Mol. weight [g/mol]:	146.18

Physical Properties

Property code	Value	Unit	Source
gf	-365.12	kJ/mol	Joback Method
hf	-590.12	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	56.62	kJ/mol	Joback Method
log10ws	-0.99		Crippen Method
logp	0.710		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
ripol	1789.00		NIST Webbook
ripol	1789.00		NIST Webbook
tb	527.59	K	Joback Method
tc	700.51	K	Joback Method
tf	286.63	K	Joback Method
vc	0.465	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.76	J/molxK	527.59	Joback Method
cpg	298.85	J/molxK	556.41	Joback Method
cpg	308.56	J/molxK	585.23	Joback Method
cpg	317.88	J/molxK	614.05	Joback Method
cpg	326.83	J/molxK	642.87	Joback Method
cpg	335.40	J/molxK	671.69	Joback Method
cpg	343.59	J/molxK	700.51	Joback Method
dvisc	0.0172601	Paxs	286.63	Joback Method

dvisc	0.0045782	Paxs	326.79	Joback Method
dvisc	0.0016237	Paxs	366.95	Joback Method
dvisc	0.0007065	Paxs	407.11	Joback Method
dvisc	0.0003570	Paxs	447.27	Joback Method
dvisc	0.0002019	Paxs	487.43	Joback Method
dvisc	0.0001245	Paxs	527.59	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=R319607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rip_{ol}:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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