

methyl 5-hydroxyhexanoate

Inchi:	InChI=1S/C7H14O3/c1-6(8)4-3-5-7(9)10-2/h6,8H,3-5H2,1-2H3
InchiKey:	KBKUVMOUCKJDBE-UHFFFAOYSA-N
Formula:	C7H14O3
SMILES:	COC(=O)CCCC(C)O
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	1827.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1827.00		NIST Webbook
tb	527.59	K	Joback Method
tc	700.51	K	Joback Method
tf	286.63	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.76	J/mol×K	527.59	Joback Method
cpg	298.85	J/mol×K	556.41	Joback Method
cpg	308.56	J/mol×K	585.23	Joback Method
cpg	317.88	J/mol×K	614.05	Joback Method
cpg	326.83	J/mol×K	642.87	Joback Method
cpg	335.40	J/mol×K	671.69	Joback Method

cpg	343.59	J/mol×K	700.51	Joback Method
dvisc	0.0172601	Pa×s	286.63	Joback Method
dvisc	0.0045782	Pa×s	326.79	Joback Method
dvisc	0.0016237	Pa×s	366.95	Joback Method
dvisc	0.0007065	Pa×s	407.11	Joback Method
dvisc	0.0003570	Pa×s	447.27	Joback Method
dvisc	0.0002019	Pa×s	487.43	Joback Method
dvisc	0.0001245	Pa×s	527.59	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R319518&Units=SI

Legend

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

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