2-Hydroxyethyl pentanoate

Inchi: InChI=1S/C7H14O3/c1-2-3-4-7(9)10-6-5-8/h8H,2-6H2,1H3
InchiKey: GFNKWCJODVREDZ-UHFFFAOYSA-N
Formula: C7H14O3
SMILES: CCCCC(=O)OCCO
Mol. weight [g/mol]: 146.18

Physical Properties

Property code	Value	Unit	Source
gf	-362.68	kJ/mol	Joback Method
hf	-584.84	kJ/mol	Joback Method
hfus	20.76	kJ/mol	Joback Method
hvap	57.01	kJ/mol	Joback Method
log10ws	-0.88		Crippen Method
logp	0.712		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1096.00		NIST Webbook
tb	528.03	K	Joback Method
tc	697.73	K	Joback Method
tf	301.63	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.44	J/mol×K	528.03	Joback Method
cpg	298.28	J/mol×K	556.31	Joback Method
cpg	307.76	J/mol×K	584.60	Joback Method
cpg	316.88	J/mol×K	612.88	Joback Method
cpg	325.65	J/mol×K	641.16	Joback Method
cpg	334.05	J/mol×K	669.45	Joback Method
cpg	342.10	J/mol×K	697.73	Joback Method
dvisc	0.0101756	Pa×s	301.63	Joback Method
dvisc	0.0032968	Pa×s	339.36	Joback Method

dvisc	0.0013384	Pa×s	377.10	Joback Method
dvisc	0.0006402	Pa×s	414.83	Joback Method
dvisc	0.0003463	Pa×s	452.56	Joback Method
dvisc	0.0002059	Pa×s	490.30	Joback Method
dvisc	0.0001318	Pa×s	528.03	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=R540539&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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