HEXANOIC ACID, 2-HYDROXY-, METHYL ESTER

Other names: 2-Hydroxycaproic acid, methyl ester
Methyl 2-hydroxycaproate
methyl 2-hydroxyhexanoate

Inchi: InChI=1S/C7H14O3/c1-3-4-5-6(8)7(9)10-2/h6,8H,3-5H2,1-2H3

InchiKey: IJQZYNRJICMGLS-UHFFFAOYSA-N

Formula: C7H14O3

SMILES: CCCCC(O)C(=O)OC

Mol. weight [g/mol]: 146.19

Physical Properties

Property code	Value	Unit	Source
hf	-673.66	kJ/mol	Cheméo Relay (1.0)
hfus	17.24	kJ/mol	Joback Method
hvap	63.75	kJ/mol	Cheméo Relay (1.0)
ie	10.17	eV	Cheméo Relay (1.0)
log10ws	-0.21		Cheméo Relay (1.0)
logp	0.710		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
ripol	1574.00		NIST Webbook
ripol	1574.00		NIST Webbook
tb	450.58	K	Cheméo Relay (1.0)
tc	643.69	K	Cheméo Relay (1.0)
tf	261.96	K	Cheméo Relay (1.0)
vc	0.461	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C68756649&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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