3-Methyl hexanoic acid

Other names: 3-methylcaproic acid
Inchi: InChI=1S/C7H14O2/c1-3-4-6(2)5-7(8)9/h6H,3-5H2,1-2H3,(H,8,9)
InchiKey: NZQMQVJXSRMTCJ-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CCCC(C)CC(=O)O
Mol. weight [g/mol]: 130.18
CAS: 3780-58-3

Physical Properties

Property code	Value	Unit	Source
gf	-260.12	kJ/mol	Joback Method
hf	-457.90	kJ/mol	Joback Method
hfus	16.05	kJ/mol	Joback Method
hvap	54.21	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.897		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
ripol	1869.00		NIST Webbook
ripol	1869.00		NIST Webbook
tb	505.17	K	Joback Method
tc	678.63	K	Joback Method
tf	264.40	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.80	J/mol×K	505.17	Joback Method
cpg	276.01	J/mol×K	534.08	Joback Method
cpg	285.78	J/mol×K	562.99	Joback Method
cpg	295.14	J/mol×K	591.90	Joback Method
cpg	304.09	J/mol×K	620.81	Joback Method
cpg	312.64	J/mol×K	649.72	Joback Method

cpg	320.81	J/mol×K	678.63	Joback Method
dvisc	0.0353274	Pa×s	264.40	Joback Method
dvisc	0.0080276	Pa×s	304.53	Joback Method
dvisc	0.0025758	Pa×s	344.66	Joback Method
dvisc	0.0010476	Pa×s	384.78	Joback Method
dvisc	0.0005050	Pa×s	424.91	Joback Method
dvisc	0.0002761	Pa×s	465.04	Joback Method
dvisc	0.0001662	Pa×s	505.17	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=C3780583&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.