HEXANOIC ACID, 2-METHYL-, METHYL ESTER

Other names: 2-Methylhexanoic acid, methyl ester
Hexanoic acid, 2-methyl, methyl ester
Inchi: InChI=1S/C8H16O2/c1-4-5-6-7(2)8(9)10-3/h7H,4-6H2,1-3H3
InchiKey: NCFJODHIQVLMQF-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CCCCC(C)C(=O)OC
Mol. weight [g/mol]: 144.21

Physical Properties

Property code	Value	Unit	Source
af	0.4689		Cheméo Relay (1.0)
gf	-219.88	kJ/mol	Joback Method
hf	-524.54	kJ/mol	Cheméo Relay (1.0)
hfus	15.74	kJ/mol	Joback Method
hvap	46.36	kJ/mol	Cheméo Relay (1.0)
ie	9.84	eV	Cheméo Relay (1.0)
log10ws	-2.23		Cheméo Relay (1.0)
logp	1.986		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	969.00		NIST Webbook
tb	406.95	K	Cheméo Relay (1.0)
tc	603.63	K	Cheméo Relay (1.0)
tf	203.36	K	Cheméo Relay (1.0)
vc	0.480	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.83	J/mol×K	458.29	Joback Method
cpg	292.41	J/mol×K	488.10	Joback Method
cpg	304.54	J/mol×K	517.91	Joback Method
cpg	316.22	J/mol×K	547.72	Joback Method
cpg	327.44	J/mol×K	577.53	Joback Method

cpg	338.23	J/mol×K	607.34	Joback Method
cpg	348.57	J/mol×K	637.16	Joback Method
dvisc	0.0048246	Pa×s	237.08	Joback Method
dvisc	0.0020946	Pa×s	273.95	Joback Method
dvisc	0.0011084	Pa×s	310.82	Joback Method
dvisc	0.0006713	Pa×s	347.69	Joback Method
dvisc	0.0004476	Pa×s	384.55	Joback Method
dvisc	0.0003204	Pa×s	421.42	Joback Method
dvisc	0.0002420	Pa×s	458.29	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2177813&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

Legend

af: Acentric Factor
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
ie: Ionization energy
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