HEXANOIC ACID, 2-OXO-, METHYL ESTER

Other names: 2-Oxo-hexanoic acid methyl ester
Inchi: InChI=1S/C7H12O3/c1-3-4-5-6(8)7(9)10-2/h3-5H2,1-2H3
InchiKey: GJIQBFATAJWGCL-UHFFFAOYSA-N
Formula: C7H12O3
SMILES: CCCCC(=O)C(=O)OC
Mol. weight [g/mol]: 144.17

Physical Properties

Property code	Value	Unit	Source
af	0.5414		Cheméo Relay (1.0)
gf	-354.78	kJ/mol	Joback Method
hf	-565.93	kJ/mol	Cheméo Relay (1.0)
hfus	18.27	kJ/mol	Joback Method
hvap	52.42	kJ/mol	Cheméo Relay (1.0)
ie	9.55	eV	Cheméo Relay (1.0)
log10ws	-1.37		Cheméo Relay (1.0)
logp	0.919		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
tb	438.46	K	Cheméo Relay (1.0)
tc	626.63	K	Cheméo Relay (1.0)
tf	263.35	K	Cheméo Relay (1.0)
vc	0.450	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.79	J/mol×K	489.72	Joback Method
cpg	266.32	J/mol×K	520.85	Joback Method
cpg	276.45	J/mol×K	551.98	Joback Method
cpg	286.16	J/mol×K	583.11	Joback Method
cpg	295.47	J/mol×K	614.24	Joback Method
cpg	304.37	J/mol×K	645.37	Joback Method
cpg	312.87	J/mol×K	676.50	Joback Method

dvisc	0.0027292	Pa×s	290.74	Joback Method
dvisc	0.0015623	Pa×s	323.90	Joback Method
dvisc	0.0009920	Pa×s	357.07	Joback Method
dvisc	0.0006804	Pa×s	390.23	Joback Method
dvisc	0.0004951	Pa×s	423.39	Joback Method
dvisc	0.0003773	Pa×s	456.56	Joback Method
dvisc	0.0002983	Pa×s	489.72	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6395831&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

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

Latest version available from: