3-OXOPENTANOIC ACID, METHYL ESTER

Other names:	Valeric acid, 3-oxo-, methyl ester
	Methyl «beta»-ketovalerate
	Methyl 3-oxopentanoate
	Methyl propionylacetate
	Methyl 3-oxo-n-valerate
	3-oxopentanoic acid methyl ester
	methyl 3-oxovalerate
Inchi:	InChI=1S/C6H10O3/c1-3-5(7)4-6(8)9-2/h3-4H2,1-2H3
InchiKey:	XJMIXEAZMCTAGH-UHFFFAOYSA-N
Formula:	C6H10O3
SMILES:	CCC(=O)CC(=O)OC
Mol. weight [g/mol]:	130.14

Physical Properties

Property code	Value	Unit	Source
af	0.4594		Cheméo Relay (1.0)
gf	-363.20	kJ/mol	Joback Method
hf	-600.37	kJ/mol	Cheméo Relay (1.0)
hfus	15.68	kJ/mol	Joback Method
hvap	48.63	kJ/mol	Cheméo Relay (1.0)
ie	9.44	eV	Cheméo Relay (1.0)
log10ws	-0.42		Cheméo Relay (1.0)
logp	0.529		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
ripol	1522.00		NIST Webbook
ripol	1522.00		NIST Webbook
ripol	1522.00		NIST Webbook
tb	441.45	K	Cheméo Relay (1.0)
tc	622.45	K	Cheméo Relay (1.0)
tf	266.35	K	Cheméo Relay (1.0)
vc	0.380	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.00	J/mol×K	466.84	Joback Method
cpg	224.34	J/mol×K	498.31	Joback Method
cpg	233.35	J/mol×K	529.78	Joback Method
cpg	242.00	J/mol×K	561.25	Joback Method
cpg	250.31	J/mol×K	592.71	Joback Method
cpg	258.27	J/mol×K	624.18	Joback Method
cpg	265.88	J/mol×K	655.65	Joback Method
dvisc	0.0026736	Pa×s	279.47	Joback Method
dvisc	0.0015646	Pa×s	310.70	Joback Method
dvisc	0.0010097	Pa×s	341.93	Joback Method
dvisc	0.0007012	Pa×s	373.15	Joback Method
dvisc	0.0005151	Pa×s	404.38	Joback Method
dvisc	0.0003956	Pa×s	435.61	Joback Method
dvisc	0.0003147	Pa×s	466.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	346.70	K	0.70	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C30414530&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume