Methyl 8-oxooctanoate

Inchi: InChI=1S/C9H16O3/c1-12-9(11)7-5-3-2-4-6-8-10/h8H,2-7H2,1H3
InchiKey: HVAXGLYKECRETN-UHFFFAOYSA-N
Formula: C9H16O3
SMILES: COC(=O)CCCCCCC=O
Mol. weight [g/mol]: 172.22
CAS: 4316-48-7

Physical Properties

Property code	Value	Unit	Source
gf	-308.54	kJ/mol	Joback Method
hf	-559.47	kJ/mol	Joback Method
hfus	24.14	kJ/mol	Joback Method
hvap	51.50	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.699		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	1334.00		NIST Webbook
tb	530.27	K	Joback Method
tc	708.91	K	Joback Method
tf	305.35	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.42	J/mol×K	530.27	Joback Method
cpg	356.63	J/mol×K	560.04	Joback Method
cpg	368.34	J/mol×K	589.82	Joback Method
cpg	379.56	J/mol×K	619.59	Joback Method
cpg	390.30	J/mol×K	649.36	Joback Method
cpg	400.56	J/mol×K	679.14	Joback Method
cpg	410.35	J/mol×K	708.91	Joback Method
dvisc	0.0030694	Pa×s	305.35	Joback Method

dvisc	0.0016586	Pa×s	342.84	Joback Method
dvisc	0.0010119	Pa×s	380.32	Joback Method
dvisc	0.0006746	Pa×s	417.81	Joback Method
dvisc	0.0004808	Pa×s	455.30	Joback Method
dvisc	0.0003608	Pa×s	492.78	Joback Method
dvisc	0.0002819	Pa×s	530.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4316487&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume