Octadecanoic acid, 2-oxo-, methyl ester

Other names: Methyl 2-oxooctadecanoate
Inchi: InChI=1S/C19H36O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(20)19(21)22-2/h3-17
InchiKey: URZVPVBICGXGEG-UHFFFAOYSA-N
Formula: C19H36O3
SMILES: CCCCCCCCCCCCCCCCC(=O)C(=O)OC
Mol. weight [g/mol]: 312.49
CAS: 2380-18-9

Physical Properties

Property code	Value	Unit	Source
gf	-253.74	kJ/mol	Joback Method
hf	-792.87	kJ/mol	Joback Method
hfus	49.35	kJ/mol	Joback Method
hvap	73.79	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.600		Crippen Method
mcvol	287.580	ml/mol	McGowan Method
pc	1162.45	kPa	Joback Method
rinpol	2213.00		NIST Webbook
rinpol	2213.00		NIST Webbook
rinpol	2213.00		NIST Webbook
tb	764.28	K	Joback Method
tc	942.71	K	Joback Method
tf	425.98	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.43	J/mol×K	764.28	Joback Method
cpg	895.45	J/mol×K	794.02	Joback Method
cpg	912.55	J/mol×K	823.76	Joback Method
cpg	928.74	J/mol×K	853.50	Joback Method
cpg	944.06	J/mol×K	883.24	Joback Method

cpg	958.51	J/mol×K	912.98	Joback Method
cpg	972.13	J/mol×K	942.71	Joback Method
dvisc	0.0013667	Pa×s	425.98	Joback Method
dvisc	0.0006490	Pa×s	482.36	Joback Method
dvisc	0.0003602	Pa×s	538.75	Joback Method
dvisc	0.0002235	Pa×s	595.13	Joback Method
dvisc	0.0001506	Pa×s	651.51	Joback Method
dvisc	0.0001081	Pa×s	707.90	Joback Method
dvisc	0.0000815	Pa×s	764.28	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2380189&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

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