Undecanoic acid, 10-oxo-, methyl ester

Other names: Methyl 10-oxoundecanoate
Inchi: InChI=1S/C12H22O3/c1-11(13)9-7-5-3-4-6-8-10-12(14)15-2/h3-10H2,1-2H3
InchiKey: TXRMRSKJQBFMRQ-UHFFFAOYSA-N
Formula: C12H22O3
SMILES: COC(=O)CCCCCCCCC(C)=O
Mol. weight [g/mol]: 214.30
CAS: 18993-09-4

Physical Properties

Property code	Value	Unit	Source
gf	-312.68	kJ/mol	Joback Method
hf	-648.39	kJ/mol	Joback Method
hfus	31.22	kJ/mol	Joback Method
hvap	58.21	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.869		Crippen Method
mcvol	188.950	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	1572.00		NIST Webbook
ripol	2200.00		NIST Webbook
tb	604.12	K	Joback Method
tc	781.95	K	Joback Method
tf	347.09	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.75	J/mol×K	604.12	Joback Method
cpg	503.49	J/mol×K	633.76	Joback Method
cpg	517.57	J/mol×K	663.40	Joback Method
cpg	531.02	J/mol×K	693.04	Joback Method
cpg	543.84	J/mol×K	722.67	Joback Method
cpg	556.04	J/mol×K	752.31	Joback Method

cpg	567.63	J/mol×K	781.95	Joback Method
dvisc	0.0024044	Pa×s	347.09	Joback Method
dvisc	0.0012547	Pa×s	389.93	Joback Method
dvisc	0.0007447	Pa×s	432.77	Joback Method
dvisc	0.0004856	Pa×s	475.61	Joback Method
dvisc	0.0003398	Pa×s	518.44	Joback Method
dvisc	0.0002511	Pa×s	561.28	Joback Method
dvisc	0.0001937	Pa×s	604.12	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18993094&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume