Decanoic acid, 9-oxo-, methyl ester

Other names: Methyl 9-oxodecanoate
Inchi: InChI=1S/C11H20O3/c1-10(12)8-6-4-3-5-7-9-11(13)14-2/h3-9H2,1-2H3
InchiKey: HBEFOKAECCZCNW-UHFFFAOYSA-N
Formula: C11H20O3
SMILES: COC(=O)CCCCCCCC(C)=O
Mol. weight [g/mol]: 200.27
CAS: 2575-07-7

Physical Properties

Property code	Value	Unit	Source
gf	-321.10	kJ/mol	Joback Method
hf	-627.75	kJ/mol	Joback Method
hfus	28.63	kJ/mol	Joback Method
hvap	55.98	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.479		Crippen Method
mcvol	174.860	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinpol	1429.00		NIST Webbook
ripol	2053.00		NIST Webbook
tb	581.24	K	Joback Method
tc	760.51	K	Joback Method
tf	335.82	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.66	J/mol×K	581.24	Joback Method
cpg	452.74	J/mol×K	611.12	Joback Method
cpg	466.22	J/mol×K	641.00	Joback Method
cpg	479.10	J/mol×K	670.88	Joback Method
cpg	491.38	J/mol×K	700.76	Joback Method
cpg	503.08	J/mol×K	730.63	Joback Method

cpg	514.20	J/mol×K	760.51	Joback Method
dvisc	0.0025267	Pa×s	335.82	Joback Method
dvisc	0.0013404	Pa×s	376.72	Joback Method
dvisc	0.0008051	Pa×s	417.63	Joback Method
dvisc	0.0005296	Pa×s	458.53	Joback Method
dvisc	0.0003732	Pa×s	499.43	Joback Method
dvisc	0.0002772	Pa×s	540.34	Joback Method
dvisc	0.0002147	Pa×s	581.24	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2575077&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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