

(E)-10-Dodecenoic acid, 9,12-dioxo, methyl ester, # 1

Inchi:	InChI=1S/C13H20O4/c1-17-13(16)10-6-4-2-3-5-8-12(15)9-7-11-14/h7,9,11H,2-6,8,10H2,
InchiKey:	NZAZBXXLAVAPII-VQHVLOKHSA-N
Formula:	C13H20O4
SMILES:	COC(=O)CCCCCCCC(=O)C=CC=O
Mol. weight [g/mol]:	240.30

Physical Properties

Property code	Value	Unit	Source
gf	-323.56	kJ/mol	Joback Method
hf	-637.39	kJ/mol	Joback Method
hfus	36.30	kJ/mol	Joback Method
hvap	67.11	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.214		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinsol	1963.00		NIST Webbook
tb	679.82	K	Joback Method
tc	866.51	K	Joback Method
tf	395.28	K	Joback Method
vc	0.790	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.58	J/molxK	679.82	Joback Method
cpg	599.85	J/molxK	835.39	Joback Method
cpg	589.13	J/molxK	804.28	Joback Method
cpg	577.76	J/molxK	773.16	Joback Method
cpg	565.72	J/molxK	742.05	Joback Method
cpg	553.01	J/molxK	710.93	Joback Method
cpg	609.96	J/molxK	866.51	Joback Method
dvisc	0.0001657	Paxs	679.82	Joback Method
dvisc	0.0002139	Paxs	632.40	Joback Method

dvisc	0.0002879	Paxs	584.97	Joback Method
dvisc	0.0004084	Paxs	537.55	Joback Method
dvisc	0.0006199	Paxs	490.13	Joback Method
dvisc	0.0010287	Paxs	442.70	Joback Method
dvisc	0.0019280	Paxs	395.28	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R554860&Units=SI

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

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