

Methyl 11-oxo-9-undecenoate

Inchi:	InChI=1S/C12H20O3/c1-15-12(14)10-8-6-4-2-3-5-7-9-11-13/h7,9,11H,2-6,8,10H2,1H3/b
InchiKey:	MGEJSRKZEJDCJG-VQHVLOKHS-A-N
Formula:	C12H20O3
SMILES:	COC(=O)CCCCCCCC=CC=O
Mol. weight [g/mol]:	212.29
CAS:	53613-55-1

Physical Properties

Property code	Value	Unit	Source
gf	-203.06	kJ/mol	Joback Method
hf	-504.17	kJ/mol	Joback Method
hfus	32.11	kJ/mol	Joback Method
hvap	58.14	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.645		Crippen Method
mvol	184.650	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1698.00		NIST Webbook
tb	603.07	K	Joback Method
tc	783.76	K	Joback Method
tf	334.08	K	Joback Method
vc	0.729	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.82	J/molxK	603.07	Joback Method
cpg	482.81	J/molxK	633.19	Joback Method
cpg	496.14	J/molxK	663.30	Joback Method
cpg	508.84	J/molxK	693.42	Joback Method
cpg	520.92	J/molxK	723.53	Joback Method
cpg	532.40	J/molxK	753.65	Joback Method
cpg	543.29	J/molxK	783.76	Joback Method
dvisc	0.0025548	Paxs	334.08	Joback Method

dvisc	0.0012682	Paxs	378.91	Joback Method
dvisc	0.0007301	Paxs	423.74	Joback Method
dvisc	0.0004672	Paxs	468.57	Joback Method
dvisc	0.0003232	Paxs	513.41	Joback Method
dvisc	0.0002372	Paxs	558.24	Joback Method
dvisc	0.0001823	Paxs	603.07	Joback Method

Sources

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=C53613551&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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