

Methyl 12-oxo-9-dodecenoate

Inchi:	InChI=1S/C13H22O3/c1-16-13(15)11-9-7-5-3-2-4-6-8-10-12-14/h6,8,12H,2-5,7,9-11H2,1
InchiKey:	QMLVRFHLQFNZEI-SOFGYWHQSA-N
Formula:	C13H22O3
SMILES:	COC(=O)CCCCCCCC=CCC=O
Mol. weight [g/mol]:	226.31
CAS:	22418-58-2

Physical Properties

Property code	Value	Unit	Source
gf	-194.64	kJ/mol	Joback Method
hf	-524.81	kJ/mol	Joback Method
hfus	34.70	kJ/mol	Joback Method
hvap	60.37	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.035		Crippen Method
mcvol	198.740	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
tb	625.95	K	Joback Method
tc	805.26	K	Joback Method
tf	345.35	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.67	J/molxK	625.95	Joback Method
cpg	585.91	J/molxK	775.38	Joback Method
cpg	573.96	J/molxK	745.49	Joback Method
cpg	561.37	J/molxK	715.61	Joback Method
cpg	548.15	J/molxK	685.72	Joback Method
cpg	534.25	J/molxK	655.84	Joback Method
cpg	597.26	J/molxK	805.26	Joback Method

dvisc	0.0001642	Paxs	625.95	Joback Method
dvisc	0.0002145	Paxs	579.18	Joback Method
dvisc	0.0002937	Paxs	532.42	Joback Method
dvisc	0.0004272	Paxs	485.65	Joback Method
dvisc	0.0006730	Paxs	438.88	Joback Method
dvisc	0.0011817	Paxs	392.12	Joback Method
dvisc	0.0024168	Paxs	345.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22418582&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

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