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/mol×K	625.95	Joback Method
cpg	534.25	J/mol×K	655.84	Joback Method
cpg	548.15	J/mol×K	685.72	Joback Method
cpg	561.37	J/mol×K	715.61	Joback Method
cpg	573.96	J/mol×K	745.49	Joback Method
cpg	585.91	J/mol×K	775.38	Joback Method
cpg	597.26	J/mol×K	805.26	Joback Method

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

Sources

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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