Dodecanedioic acid, dimethyl ester

Other names:	1,12-Dimethyl dodecanedioate
	Dimethyl 1,10-decanedicarboxylate
	Dimethyl 1,12-dodecanedioate
	Dimethyl dodecanedioate
	dimethyl 1,12-dodecanoate
	dimethyl dodecanoate
	dodecanedioic acid dimethyl ester
Inchi:	InChI=1S/C14H26O4/c1-17-13(15)11-9-7-5-3-4-6-8-10-12-14(16)18-2/h3-12H2,1-2H3
InchiKey:	IZMOTZDBVPMOFE-UHFFFAOYSA-N
Formula:	C14H26O4
SMILES:	COC(=O)CCCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	258.35
CAS:	1731-79-9

Physical Properties

Property code	Value	Unit	Source
gf	-400.84	kJ/mol	Joback Method
hf	-821.89	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	65.07	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.233		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	1853.70		NIST Webbook
rinpol	1851.00		NIST Webbook
rinpol	1853.70		NIST Webbook
rinpol	309.45		NIST Webbook
rinpol	309.45		NIST Webbook
rinpol	1851.00		NIST Webbook
tb	672.30	K	Joback Method
tc	848.26	K	Joback Method
tf	391.86	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.19	J/mol×K	672.30	Joback Method
cpg	637.83	J/mol×K	701.63	Joback Method
cpg	652.75	J/mol×K	730.95	Joback Method
cpg	666.95	J/mol×K	760.28	Joback Method
cpg	680.44	J/mol×K	789.61	Joback Method
cpg	693.22	J/mol×K	818.93	Joback Method
cpg	705.29	J/mol×K	848.26	Joback Method
dvisc	0.0001198	Pa×s	672.30	Joback Method
dvisc	0.0007810	Pa×s	438.60	Joback Method
dvisc	0.0014859	Pa×s	391.86	Joback Method
dvisc	0.0003028	Pa×s	532.08	Joback Method
dvisc	0.0002115	Pa×s	578.82	Joback Method
dvisc	0.0001558	Pa×s	625.56	Joback Method
dvisc	0.0004646	Pa×s	485.34	Joback Method
rhol	959.40	kg/m3	313.15	Phase Equilibria for the Hydroesterification of 10-Undecenoic Acid Methyl Ester
rhol	951.00	kg/m3	323.15	Phase Equilibria for the Hydroesterification of 10-Undecenoic Acid Methyl Ester
rhol	943.10	kg/m3	333.15	Phase Equilibria for the Hydroesterification of 10-Undecenoic Acid Methyl Ester
rhol	934.40	kg/m3	343.15	Phase Equilibria for the Hydroesterification of 10-Undecenoic Acid Methyl Ester
rhol	927.00	kg/m3	352.15	Phase Equilibria for the Hydroesterification of 10-Undecenoic Acid Methyl Ester

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	441.20	K	1.00	NIST Webbook
tbrp	460.50 ± 0.50	K	1.90	NIST Webbook

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=C1731799&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Phase Equilibria for the Hydroesterification of 10-Undecenoic Acid Methyl Ester:	https://www.doi.org/10.1021/acs.jced.6b00360

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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume