Octanedioic acid, dimethyl ester

Other names:	1,8-octanedioic acid, dimethyl ester
	Dimethyl ester of octanedioic acid
	Octandioic acid, dimethyl ester
	dimethyl octanedioate
	dimethyl suberate
	suberic acid, dimethyl ester
Inchi:	InChI=1S/C10H18O4/c1-13-9(11)7-5-3-4-6-8-10(12)14-2/h3-8H2,1-2H3
InchiKey:	LNLCRJXCNQABMV-UHFFFAOYSA-N
Formula:	C10H18O4
SMILES:	COC(=O)CCCCCCC(=O)OC
Mol. weight [g/mol]:	202.25
CAS:	1732-09-8

Physical Properties

Property code	Value	Unit	Source
chs	-5574.30	kJ/mol	NIST Webbook
gf	-434.52	kJ/mol	Joback Method
hf	-739.33	kJ/mol	Joback Method
hfus	27.23	kJ/mol	Joback Method
hvap	78.10 ± 0.20	kJ/mol	NIST Webbook
log10ws	-1.73		Crippen Method
logp	1.673		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2300.00	kPa	Vapor Pressures, Enthalpies of Vaporization, and Critical Parameters of a Series of Linear Aliphatic Dimethyl Esters of Dicarboxylic Acids
rinpol	1409.00		NIST Webbook
rinpol	247.42		NIST Webbook
rinpol	249.30		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	249.30		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1448.00		NIST Webbook

rinpol	1448.00		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1447.30		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	249.30		NIST Webbook
ripol	2010.00		NIST Webbook
ripol	2010.00		NIST Webbook
ripol	1985.00		NIST Webbook
ripol	2010.00		NIST Webbook
ripol	2010.00		NIST Webbook
ripol	1973.00		NIST Webbook
tb	541.20	K	NIST Webbook
tc	760.87	K	Joback Method
tf	346.78	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.69	J/mol×K	580.78	Joback Method
cpg	428.88	J/mol×K	610.80	Joback Method
cpg	441.54	J/mol×K	640.81	Joback Method
cpg	453.66	J/mol×K	670.83	Joback Method
cpg	465.23	J/mol×K	700.84	Joback Method
cpg	476.26	J/mol×K	730.86	Joback Method
cpg	486.74	J/mol×K	760.87	Joback Method
dvisc	0.0019074	Pa×s	346.78	Joback Method

dvisc	0.0010682	Pa×s	385.78	Joback Method
dvisc	0.0006655	Pa×s	424.78	Joback Method
dvisc	0.0004489	Pa×s	463.78	Joback Method
dvisc	0.0003219	Pa×s	502.78	Joback Method
dvisc	0.0002421	Pa×s	541.78	Joback Method
dvisc	0.0001892	Pa×s	580.78	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	419.50 ± 1.50	K	2.40	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=C1732098&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressures, Enthalpies of Vaporization, and Critical Parameters of a Series of Linear Aliphatic Dimethyl Esters of Dicarboxylic Acids:	https://www.doi.org/10.1021/je0602418

Legend

chs:	Standard solid enthalpy of combustion
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

ripol:	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

Latest version available from:
https://www.chemeo.com/cid/21-265-4/Octanedioic-acid-dimethyl-ester.pdf
Generated by Cheméo on 2025-12-22 01:39:41.82512504 +0000 UTC m=+6115779.355165693.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.