Diethyl suberate

Other names:	1,8-octanedioic acid, diethyl ester
	Diethyl octanedioate
	Ethyl suberate
	Octanedioic acid, diethyl ester
	diethyl 1,8-octanedioate
	suberic acid, diethyl ester
Inchi:	InChI=1S/C12H22O4/c1-3-15-11(13)9-7-5-6-8-10-12(14)16-4-2/h3-10H2,1-2H3
InchiKey:	PEUGOJXLBSIJQS-UHFFFAOYSA-N
Formula:	C12H22O4
SMILES:	CCOC(=O)CCCCCCC(=O)OCC
Mol. weight [g/mol]:	230.30
CAS:	2050-23-9

Physical Properties

Property code	Value	Unit	Source
gf	-417.68	kJ/mol	Joback Method
hf	-780.61	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-2.53		Aqueous Solubility Prediction Method
logp	2.453		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1552.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1552.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1583.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2114.00		NIST Webbook
tb	555.80	K	NIST Webbook
tc	723.00	K	Vapor-liquid critical temperatures and pressures of dicarboxylic acid diethyl esters

tf	279.05	K	Aqueous Solubility Prediction Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.96	J/mol×K	626.54	Joback Method
cpg	582.39	J/mol×K	774.35	Joback Method
cpg	570.37	J/mol×K	744.79	Joback Method
cpg	557.71	J/mol×K	715.23	Joback Method
cpg	544.42	J/mol×K	685.66	Joback Method
cpg	530.51	J/mol×K	656.10	Joback Method
cpg	593.78	J/mol×K	803.91	Joback Method
dvisc	0.0001522	Pa×s	626.54	Joback Method
dvisc	0.0001965	Pa×s	583.67	Joback Method
dvisc	0.0002641	Pa×s	540.80	Joback Method
dvisc	0.0003735	Pa×s	497.93	Joback Method
dvisc	0.0005638	Pa×s	455.06	Joback Method
dvisc	0.0009273	Pa×s	412.19	Joback Method
dvisc	0.0017118	Pa×s	369.32	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2050239&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Vapor-liquid critical temperatures and pressures of dicarboxylic acid diethyl esters: https://www.doi.org/10.1016/j.jct.2017.09.004

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