1,4-Benzenedicarboxylic acid, diethyl ester

Other names:	Terephthalic acid, diethyl ester
	Diethyl terephthalate
	Diethyl ester of 1,4-Benzenedicarboxylic acid
	Diethyl p-phthalate
Inchi:	InChI=1S/C12H14O4/c1-3-15-11(13)9-5-7-10(8-6-9)12(14)16-4-2/h5-8H,3-4H2,1-2H3
InchiKey:	ONIHPYYWNBVMID-UHFFFAOYSA-N
Formula:	C12H14O4
SMILES:	CCOC(=O)c1ccc(C(=O)OCC)cc1
Mol. weight [g/mol]:	222.24
CAS:	636-09-9

Physical Properties

Property code	Value	Unit	Source
gf	-314.90	kJ/mol	Joback Method
hf	-555.55	kJ/mol	Joback Method
hfus	26.06	kJ/mol	Joback Method
hvap	63.56	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.040		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	1613.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1650.00		NIST Webbook
tb	575.15 ± 1.00	K	NIST Webbook
tc	870.02	K	Joback Method
tf	317.00	K	NIST Webbook
tf	316.35 ± 0.60	K	NIST Webbook
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.51	J/mol×K	658.20	Joback Method
cpg	495.18	J/mol×K	834.72	Joback Method
cpg	485.06	J/mol×K	799.41	Joback Method
cpg	474.13	J/mol×K	764.11	Joback Method
cpg	462.40	J/mol×K	728.81	Joback Method
cpg	449.86	J/mol×K	693.50	Joback Method
cpg	504.49	J/mol×K	870.02	Joback Method
cpl	381.00	J/mol×K	320.00	NIST Webbook
dvisc	0.0011118	Pa×s	408.26	Joback Method
dvisc	0.0001492	Pa×s	658.20	Joback Method
dvisc	0.0001863	Pa×s	616.54	Joback Method
dvisc	0.0002401	Pa×s	574.89	Joback Method
dvisc	0.0003219	Pa×s	533.23	Joback Method
dvisc	0.0004537	Pa×s	491.57	Joback Method
dvisc	0.0006814	Pa×s	449.92	Joback Method
hfust	24.69	kJ/mol	317.20	NIST Webbook
hfust	24.69	kJ/mol	317.20	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.20	K	0.30	NIST Webbook
tbrp	415.00	K	0.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C636099&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
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume