1,4-Benzenedicarboxylic acid, dimethyl ester

Other names: 1,4-Benzenedicarboxylic acid dimethyl ester
1,4-Benzenedicarboxylic acid, 1,4-dimethyl ester
DIMETHYL 1,4-BENZENEDICARBOXYLATE
DIMETHYL P-PHTHALATE
DMT
Dimethyl ester of 1,4-benzenedicarboxylic acid
Dimethyl p-benzenedicarboxylate
Dimethyl terephthalate
Dimethyl terphthalate
Dimethylester kyseliny isoftalove
Dimethylester kyseliny tereftalove
METHYL 4-(CARBOMETHOXY)BENZOATE
Methyl p-(methoxycarbonyl)benzoate
NCI-C50055
NSC 3503
Terephthalate, dimethyl
Terephthalic acid, dimethyl ester
dimethyl benzene-1,4-dicarboxylate

Inchi: InChI=1S/C10H10O4/c1-13-9(11)7-3-5-8(6-4-7)10(12)14-2/h3-6H,1-2H3
InchiKey: WOZVHXUHUFLZGK-UHFFFAOYSA-N
Formula: C10H10O4
SMILES: COC(=O)c1ccc(C(=O)OC)cc1
Mol. weight [g/mol]: 194.18
CAS: 120-61-6

Physical Properties

Property code	Value	Unit	Source
affp	843.20	kJ/mol	NIST Webbook
basg	812.30	kJ/mol	NIST Webbook
chs	-4631.66 ± 0.88	kJ/mol	NIST Webbook
ea	0.64	eV	NIST Webbook
ea	0.82 ± 0.09	eV	NIST Webbook
ea	0.82 ± 0.09	eV	NIST Webbook
gf	-331.74	kJ/mol	Joback Method
hf	-514.27	kJ/mol	Joback Method
hfs	-710.00	kJ/mol	NIST Webbook
hfs	-732.60 ± 1.00	kJ/mol	NIST Webbook

hfus	33.01	kJ/mol	Thermal analysis of phase change materials in the temperature range 120.150 .C
hsub	104.60 ± 0.30	kJ/mol	NIST Webbook
hsub	104.60 ± 0.30	kJ/mol	NIST Webbook
hvap	59.10	kJ/mol	Joback Method
ie	9.78 ± 0.03	eV	NIST Webbook
log10ws	-3.72		Aqueous Solubility Prediction Method
logp	1.260		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
rinpol	1512.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1468.00		NIST Webbook
tb	612.44	K	Joback Method
tc	831.50	K	Joback Method
tf	413.80 ± 0.01	K	NIST Webbook
tf	414.40	K	Aqueous Solubility Prediction Method
tf	413.00 ± 4.00	K	NIST Webbook
tf	413.80 ± 0.20	K	NIST Webbook
tf	413.00 ± 1.50	K	NIST Webbook
tf	415.20 ± 0.20	K	NIST Webbook
tt	413.88	K	Solubility and Thermodynamic Modeling of Dimethyl Terephthalate in Pure Solvents and the Evaluation of the Mixing Properties of the Solutions
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.66	J/mol×K	831.50	Joback Method
cpg	382.23	J/mol×K	758.48	Joback Method
cpg	391.31	J/mol×K	794.99	Joback Method
cpg	338.80	J/mol×K	612.44	Joback Method
cpg	350.71	J/mol×K	648.95	Joback Method
cpg	361.93	J/mol×K	685.46	Joback Method
cpg	372.43	J/mol×K	721.97	Joback Method
cps	276.10	J/mol×K	353.00	NIST Webbook
cps	261.10	J/mol×K	298.15	NIST Webbook
dvisc	0.0002869	Pa×s	536.87	Joback Method
dvisc	0.0002254	Pa×s	574.65	Joback Method
dvisc	0.0001824	Pa×s	612.44	Joback Method
dvisc	0.0012091	Pa×s	385.72	Joback Method
dvisc	0.0007664	Pa×s	423.51	Joback Method
dvisc	0.0005235	Pa×s	461.29	Joback Method
dvisc	0.0003788	Pa×s	499.08	Joback Method
hfust	32.09	kJ/mol	413.80	NIST Webbook
hfust	31.63	kJ/mol	413.79	NIST Webbook
hfust	32.10	kJ/mol	413.80	NIST Webbook
hfust	32.00	kJ/mol	415.40	NIST Webbook
hsubt	94.40	kJ/mol	393.00	NIST Webbook
hsubt	88.30	kJ/mol	393.00	NIST Webbook
hsubt	103.80 ± 0.30	kJ/mol	320.50	NIST Webbook
hvapt	62.00	kJ/mol	468.00	NIST Webbook
sfust	77.60	J/mol×K	413.80	NIST Webbook
sfust	76.44	J/mol×K	413.79	NIST Webbook
sfust	77.00	J/mol×K	415.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50856e+01
Coeff. B	-4.51226e+03
Coeff. C	-1.26067e+02

Temperature range (K), min.	430.99
Temperature range (K), max.	587.72

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.91810e+01
Coeff. B	-9.27175e+03
Coeff. C	-6.14065e+00
Coeff. D	2.66169e-06
Temperature range (K), min.	403.80
Temperature range (K), max.	772.00

Sources

Solubility and Thermodynamic Modeling of Dimethyl Terephthalate in Pure Solvents and the Evaluation of the Mixing Properties of the Solutions:	https://www.doi.org/10.1021/acs.jced.9b00658
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermal analysis of phase change materials in the temperature range 120-150 .C:	https://www.doi.org/10.1016/j.tca.2010.11.011
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1148.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120616&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1148
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions

hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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