1,3-Benzenedicarboxylic acid, dimethyl ester

Other names:	1,3-Benzenedicarboxylic acid, 1,3-dimethyl ester
	DIMETHYL 1,3-BENZENEDICARBOXYLATE
	DIMETHYL M-PHTHALATE
	Dimethyl benzene-1,3-dicarboxylate
	Dimethyl isophthalate
	Dimethylester kyseliny isoftalove
	Dimethylester kyseliny tereftalove
	Isophthalic acid, dimethyl ester
	Methyl 3-(carbomethoxy)benzoate
	Methyl isophthalate
	Morflex 1129
	NSC 15313
	Uniplex 270
Inchi:	InChI=1S/C10H10O4/c1-13-9(11)7-4-3-5-8(6-7)10(12)14-2/h3-6H,1-2H3
InchiKey:	VNGOYPQMJFJDLV-UHFFFAOYSA-N
Formula:	C10H10O4
SMILES:	COC(=O)c1cccc(C(=O)OC)c1
Mol. weight [g/mol]:	194.18
CAS:	1459-93-4

Physical Properties

Property code	Value	Unit	Source
affp	843.50	kJ/mol	NIST Webbook
basg	814.30	kJ/mol	NIST Webbook
chs	-4633.37 ± 0.88	kJ/mol	NIST Webbook
chs	-4634.20 ± 1.50	kJ/mol	NIST Webbook
ea	0.55	eV	NIST Webbook
gf	-331.74	kJ/mol	Joback Method
hf	-629.20 ± 2.00	kJ/mol	NIST Webbook
hf	-630.00	kJ/mol	NIST Webbook
hfs	-730.10 ± 2.00	kJ/mol	NIST Webbook
hfs	-730.90 ± 1.00	kJ/mol	NIST Webbook
hfus	20.88	kJ/mol	Joback Method
hsub	100.90	kJ/mol	NIST Webbook
hsub	100.90 ± 0.20	kJ/mol	NIST Webbook
hsub	100.70	kJ/mol	NIST Webbook
hsub	100.90 ± 0.20	kJ/mol	NIST Webbook

hvap	77.20 ± 0.80	kJ/mol	NIST Webbook
ie	9.84 ± 0.09	eV	NIST Webbook
log10ws	-1.96		Crippen Method
logp	1.260		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	2650.00 ± 200.00	kPa	NIST Webbook
rhoc	341.96 ± 25.24	kg/m3	NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	256.92		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1488.00		NIST Webbook
tb	555.00	K	NIST Webbook
tb	555.20	K	NIST Webbook
tc	766.00 ± 6.00	K	NIST Webbook
tf	341.15 ± 0.25	K	NIST Webbook
tf	340.70 ± 0.20	K	NIST Webbook
tt	341.50 ± 0.30	K	NIST Webbook
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	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
cpg	382.23	J/mol×K	758.48	Joback Method
cpg	391.31	J/mol×K	794.99	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
dvisc	0.0002869	Pa×s	536.87	Joback Method
dvisc	0.0002254	Pa×s	574.65	Joback Method
hfust	25.30	kJ/mol	341.20	NIST Webbook
hsubt	100.70 ± 0.20	kJ/mol	302.00	NIST Webbook
hvapt	60.50	kJ/mol	471.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	397.20	K	1.60	NIST Webbook
tbrp	397.00	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42560e+01
Coeff. B	-3.58033e+03
Coeff. C	-1.51505e+02
Temperature range (K), min.	402.65
Temperature range (K), max.	551.79

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.16028e+02
Coeff. B	-1.74767e+04
Coeff. C	-2.93749e+01
Coeff. D	1.88069e-05
Temperature range (K), min.	358.15
Temperature range (K), max.	426.15

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1147.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1459934&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1147
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
rhoc:	Critical 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
tt:	Triple Point Temperature
vc:	Critical Volume