1,4-Benzenedicarboxylic acid, 2-hydroxy-, 1,4-dimethyl ester

Other names: 1,4-Benzenedicarboxylic acid, 2-hydroxy-, dimethyl ester
Terephthalic acid, hydroxy-, dimethyl ester
Dimethyl 2-hydroxyterephthalate
Dimethyl hydroxyterephthalate
Hydroxyterephthalic acid dimethyl ester
NSC 46640
Benzene-1,4-dicarboxylic acid, 2-hydroxy, dimethyl ester

Inchi: InChI=1S/C10H10O5/c1-14-9(12)6-3-4-7(8(11)5-6)10(13)15-2/h3-5,11H,1-2H3

InchiKey: CJOJIAKIRLKBOO-UHFFFAOYSA-N

Formula: C10H10O5

SMILES: COC(=O)c1ccc(C(=O)OC)c(O)c1

Mol. weight [g/mol]: 210.18

CAS: 6342-72-9

Physical Properties

Property code	Value	Unit	Source
gf	-486.36	kJ/mol	Joback Method
hf	-691.58	kJ/mol	Joback Method
hfus	26.67	kJ/mol	Joback Method
hvap	72.12	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	0.965		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	1586.00		NIST Webbook
rinpol	1625.70		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1625.70		NIST Webbook
tb	693.06	K	Joback Method
tc	920.77	K	Joback Method
tf	497.44	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.57	J/mol×K	693.06	Joback Method
cpg	429.52	J/mol×K	882.82	Joback Method
cpg	421.52	J/mol×K	844.87	Joback Method
cpg	412.96	J/mol×K	806.92	Joback Method
cpg	403.80	J/mol×K	768.96	Joback Method
cpg	394.02	J/mol×K	731.01	Joback Method
cpg	437.01	J/mol×K	920.77	Joback Method
dvisc	0.0000171	Pa×s	693.06	Joback Method
dvisc	0.0000235	Pa×s	660.46	Joback Method
dvisc	0.0000334	Pa×s	627.85	Joback Method
dvisc	0.0000494	Pa×s	595.25	Joback Method
dvisc	0.0000764	Pa×s	562.65	Joback Method
dvisc	0.0001248	Pa×s	530.04	Joback Method
dvisc	0.0002172	Pa×s	497.44	Joback Method

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=C6342729&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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