1,3-Benzenedicarboxylic acid, 4-methyl-, dimethyl ester

Other names: Dimethyl 4-methyl-1,3-benzenedicarboxylate
Dimethyl 4-methylisophthalate
Isophthalic acid, 4-methyl-, dimethyl ester

Inchi: InChI=1S/C11H12O4/c1-7-4-5-8(10(12)14-2)6-9(7)11(13)15-3/h4-6H,1-3H3

InchiKey: MTDRWWFCMSDTBL-UHFFFAOYSA-N

Formula: C11H12O4

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

Mol. weight [g/mol]: 208.21

CAS: 23038-61-1

Physical Properties

Property code	Value	Unit	Source
gf	-332.95	kJ/mol	Joback Method
hf	-546.38	kJ/mol	Joback Method
hfus	23.08	kJ/mol	Joback Method
hvap	61.99	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	1.568		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
tb	640.30	K	Joback Method
tc	856.49	K	Joback Method
tf	409.51	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.86	J/mol×K	640.30	Joback Method
cpg	398.36	J/mol×K	676.33	Joback Method
cpg	410.14	J/mol×K	712.36	Joback Method
cpg	421.20	J/mol×K	748.40	Joback Method
cpg	431.51	J/mol×K	784.43	Joback Method
cpg	441.07	J/mol×K	820.46	Joback Method

cpg	449.88	J/mol×K	856.49	Joback Method
dvisc	0.0009633	Pa×s	409.51	Joback Method
dvisc	0.0006315	Pa×s	447.97	Joback Method
dvisc	0.0004426	Pa×s	486.44	Joback Method
dvisc	0.0003268	Pa×s	524.90	Joback Method
dvisc	0.0002515	Pa×s	563.37	Joback Method
dvisc	0.0002001	Pa×s	601.84	Joback Method
dvisc	0.0001637	Pa×s	640.30	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=C23038611&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume