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

Other names: Dimethyl 2-bromoterephthalate
Inchi: InChI=1S/C10H9BrO4/c1-14-9(12)6-3-4-7(8(11)5-6)10(13)15-2/h3-5H,1-2H3
InchiKey: VUMPFOPENBVFOF-UHFFFAOYSA-N
Formula: C10H9BrO4
SMILES: COC(=O)c1ccc(C(=O)OC)c(Br)c1
Mol. weight [g/mol]: 273.08
CAS: 18643-86-2

Physical Properties

Property code	Value	Unit	Source
gf	-327.05	kJ/mol	Joback Method
hf	-499.41	kJ/mol	Joback Method
hfus	25.78	kJ/mol	Joback Method
hvap	66.20	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.022		Crippen Method
mcvol	160.380	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
tb	683.58	K	Joback Method
tc	914.90	K	Joback Method
tf	458.04	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.20	J/mol×K	683.58	Joback Method
cpg	415.60	J/mol×K	876.35	Joback Method
cpg	408.03	J/mol×K	837.79	Joback Method
cpg	399.69	J/mol×K	799.24	Joback Method
cpg	390.61	J/mol×K	760.69	Joback Method
cpg	380.78	J/mol×K	722.13	Joback Method
cpg	422.41	J/mol×K	914.90	Joback Method
dvisc	0.0001690	Pa×s	683.58	Joback Method

dvisc	0.0002039	Pa×s	645.99	Joback Method
dvisc	0.0002517	Pa×s	608.40	Joback Method
dvisc	0.0003196	Pa×s	570.81	Joback Method
dvisc	0.0004196	Pa×s	533.22	Joback Method
dvisc	0.0005740	Pa×s	495.63	Joback Method
dvisc	0.0008269	Pa×s	458.04	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=C18643862&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