

1,3-Benzenedicarboxylic acid, 5-bromo-, dimethyl ester

Other names:	dimethyl 5-bromoisophthalate
Inchi:	InChI=1S/C10H9BrO4/c1-14-9(12)6-3-7(10(13)15-2)5-8(11)4-6/h3-5H,1-2H3
InchiKey:	QUJINGKSNJNXEB-UHFFFAOYSA-N
Formula:	C10H9BrO4
SMILES:	COC(=O)c1cc(Br)cc(C(=O)OC)c1
Mol. weight [g/mol]:	273.08
CAS:	51760-21-5

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/molxK	683.58	Joback Method
cpg	380.78	J/molxK	722.13	Joback Method
cpg	390.61	J/molxK	760.69	Joback Method
cpg	399.69	J/molxK	799.24	Joback Method
cpg	408.03	J/molxK	837.79	Joback Method
cpg	415.60	J/molxK	876.35	Joback Method
cpg	422.41	J/molxK	914.90	Joback Method
dvisc	0.0008269	Paxs	458.04	Joback Method

dvisc	0.0005740	Paxs	495.63	Joback Method
dvisc	0.0004196	Paxs	533.22	Joback Method
dvisc	0.0003196	Paxs	570.81	Joback Method
dvisc	0.0002517	Paxs	608.40	Joback Method
dvisc	0.0002039	Paxs	645.99	Joback Method
dvisc	0.0001690	Paxs	683.58	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C51760215&Units=SI

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

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