1,2-Benzenedicarboxylic acid, 4-bromo-

Other names: 4-bromophthalic acid
Inchi: InChI=1S/C8H5BrO4/c9-4-1-2-5(7(10)11)6(3-4)8(12)13/h1-3H,(H,10,11)(H,12,13)
InchiKey: AZXKGUVDIORSED-UHFFFAOYSA-N
Formula: C8H5BrO4
SMILES: O=C(O)c1ccc(Br)cc1C(=O)O
Mol. weight [g/mol]: 245.03
CAS: 6968-28-1

Physical Properties

Property code	Value	Unit	Source
gf	-407.53	kJ/mol	Joback Method
hf	-498.15	kJ/mol	Joback Method
hfus	26.40	kJ/mol	Joback Method
hvap	90.29	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	1.845		Crippen Method
mcvol	132.200	ml/mol	McGowan Method
pc	5862.92	kPa	Joback Method
tb	777.34	K	Joback Method
tc	989.86	K	Joback Method
tf	512.68	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.78	J/mol×K	777.34	Joback Method
cpg	309.29	J/mol×K	812.76	Joback Method
cpg	314.37	J/mol×K	848.18	Joback Method
cpg	319.05	J/mol×K	883.60	Joback Method
cpg	323.35	J/mol×K	919.02	Joback Method
cpg	327.30	J/mol×K	954.44	Joback Method
cpg	330.92	J/mol×K	989.86	Joback Method
dvisc	0.0004271	Pa×s	512.68	Joback Method

dvisc	0.0001909	Pa×s	556.79	Joback Method
dvisc	0.0000960	Pa×s	600.90	Joback Method
dvisc	0.0000531	Pa×s	645.01	Joback Method
dvisc	0.0000316	Pa×s	689.12	Joback Method
dvisc	0.0000201	Pa×s	733.23	Joback Method
dvisc	0.0000134	Pa×s	777.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6968281&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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