4-Bromophthalic acid, anhydride

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

Physical Properties

Property code	Value	Unit	Source
hf	-609.09	kJ/mol	Cheméo Relay (1.0)
hfus	26.40	kJ/mol	Joback Method
ie	9.59	eV	Cheméo Relay (1.0)
log10ws	-2.81		Cheméo Relay (1.0)
logp	1.845		Crippen Method
mcvol	132.200	ml/mol	McGowan Method
tb	578.72	K	Cheméo Relay (1.0)
tf	443.19	K	Cheméo Relay (1.0)

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point