2-Bromo-benzoic acid biphenyl-4-yl ester

Other names: 2-Bromobenzoic acid, 4-biphenyl ester
Inchi: InChI=1S/C19H13BrO2/c20-18-9-5-4-8-17(18)19(21)22-16-12-10-15(11-13-16)14-6-2-1-3
InchiKey: ZREUHIFWVAMBSH-UHFFFAOYSA-N
Formula: C19H13BrO2
SMILES: O=C(Oc1ccc(-c2ccccc2)cc1)c1ccccc1Br
Mol. weight [g/mol]: 353.21
CAS: 301208-68-4

Physical Properties

Property code	Value	Unit	Source
gf	207.47	kJ/mol	Joback Method
hf	32.69	kJ/mol	Joback Method
hfus	34.38	kJ/mol	Joback Method
hvap	81.63	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	5.335		Crippen Method
mcvol	232.230	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	2899.00		NIST Webbook
tb	866.57	K	Joback Method
tc	1138.77	K	Joback Method
tf	540.15	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.58	J/mol×K	866.57	Joback Method
cpg	633.40	J/mol×K	911.94	Joback Method
cpg	644.85	J/mol×K	957.30	Joback Method
cpg	655.06	J/mol×K	1002.67	Joback Method
cpg	664.14	J/mol×K	1048.04	Joback Method
cpg	672.21	J/mol×K	1093.41	Joback Method
cpg	679.40	J/mol×K	1138.77	Joback Method

dvisc	0.0005089	Pa×s	540.15	Joback Method
dvisc	0.0003194	Pa×s	594.55	Joback Method
dvisc	0.0002167	Pa×s	648.96	Joback Method
dvisc	0.0001561	Pa×s	703.36	Joback Method
dvisc	0.0001179	Pa×s	757.76	Joback Method
dvisc	0.0000925	Pa×s	812.17	Joback Method
dvisc	0.0000748	Pa×s	866.57	Joback Method

Sources

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=C301208684&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume