

3-Bromobenzoic acid, 4-biphenyl ester

Inchi: InChI=1S/C19H13BrO2/c20-17-8-4-7-16(13-17)19(21)22-18-11-9-15(10-12-18)14-5-2-1-3
InchiKey: HHUWNSSMBHPCEF-UHFFFAOYSA-N
Formula: C19H13BrO2
SMILES: O=C(Oc1ccc(-c2ccccc2)cc1)c1cccc(Br)c1
Mol. weight [g/mol]: 353.21

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	2904.00		NIST Webbook
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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/molxK	866.57	Joback Method
cpg	672.21	J/molxK	1093.41	Joback Method
cpg	664.14	J/molxK	1048.04	Joback Method
cpg	655.06	J/molxK	1002.67	Joback Method
cpg	644.85	J/molxK	957.30	Joback Method
cpg	633.40	J/molxK	911.94	Joback Method
cpg	679.40	J/molxK	1138.77	Joback Method
dvisc	0.0000748	Paxs	866.57	Joback Method

dvisc	0.0000925	Paxs	812.17	Joback Method
dvisc	0.0001179	Paxs	757.76	Joback Method
dvisc	0.0001561	Paxs	703.36	Joback Method
dvisc	0.0002167	Paxs	648.96	Joback Method
dvisc	0.0003194	Paxs	594.55	Joback Method
dvisc	0.0005089	Paxs	540.15	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=U355190&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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