2-Bromobenzoic acid, 2-isopropoxyphenyl ester

Inchi: InChI=1S/C16H15BrO3/c1-11(2)19-14-9-5-6-10-15(14)20-16(18)12-7-3-4-8-13(12)17/h3-

InchiKey: LOLOAAHMLKVPBH-UHFFFAOYSA-N

Formula: C16H15BrO3

SMILES: CC(C)Oc1ccccc1OC(=O)c1ccccc1Br

Mol. weight [g/mol]: 335.19

Physical Properties

Property code	Value	Unit	Source
gf	-37.64	kJ/mol	Joback Method
hf	-279.42	kJ/mol	Joback Method
hfus	30.24	kJ/mol	Joback Method
hvap	74.70	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.455		Crippen Method
mcvol	219.590	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
rinpol	2148.00		NIST Webbook
rinpol	2148.00		NIST Webbook
tb	793.23	K	Joback Method
tc	1038.51	K	Joback Method
tf	487.15	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.21	J/mol×K	793.23	Joback Method
cpg	593.93	J/mol×K	834.11	Joback Method
cpg	606.40	J/mol×K	874.99	Joback Method
cpg	617.68	J/mol×K	915.87	Joback Method
cpg	627.79	J/mol×K	956.75	Joback Method
cpg	636.79	J/mol×K	997.63	Joback Method
cpg	644.71	J/mol×K	1038.51	Joback Method
dvisc	0.0005868	Pa×s	487.15	Joback Method

dvisc	0.0003542	Pa×s	538.16	Joback Method
dvisc	0.0002333	Pa×s	589.18	Joback Method
dvisc	0.0001643	Pa×s	640.19	Joback Method
dvisc	0.0001218	Pa×s	691.20	Joback Method
dvisc	0.0000941	Pa×s	742.22	Joback Method
dvisc	0.0000752	Pa×s	793.23	Joback Method

Sources

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=U299019&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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