

3-Bromobenzoic acid, 2-isopropoxyphenyl ester

Inchi:	InChI=1S/C16H15BrO3/c1-11(2)19-14-8-3-4-9-15(14)20-16(18)12-6-5-7-13(17)10-12/h3
InchiKey:	YJXMKPVDGNZSRJ-UHFFFAOYSA-N
Formula:	C16H15BrO3
SMILES:	CC(C)Oc1ccccc1OC(=O)c1cccc(Br)c1
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	2175.50		NIST Webbook
rinpol	2175.50		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/molxK	793.23	Joback Method
cpg	593.93	J/molxK	834.11	Joback Method
cpg	606.40	J/molxK	874.99	Joback Method
cpg	617.68	J/molxK	915.87	Joback Method
cpg	627.79	J/molxK	956.75	Joback Method
cpg	636.79	J/molxK	997.63	Joback Method
cpg	644.71	J/molxK	1038.51	Joback Method
dvisc	0.0005868	Paxs	487.15	Joback Method

dvisc	0.0003542	Paxs	538.16	Joback Method
dvisc	0.0002333	Paxs	589.18	Joback Method
dvisc	0.0001643	Paxs	640.19	Joback Method
dvisc	0.0001218	Paxs	691.20	Joback Method
dvisc	0.0000941	Paxs	742.22	Joback Method
dvisc	0.0000752	Paxs	793.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292667&Units=SI
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

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
mccvol:	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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