2-Bromobenzoic acid, 2-propylphenyl ester

Inchi: InChI=1S/C16H15BrO2/c1-2-7-12-8-3-6-11-15(12)19-16(18)13-9-4-5-10-14(13)17/h3-6,8
InchiKey: WEVCSWPQSUXKDV-UHFFFAOYSA-N
Formula: C16H15BrO2
SMILES: CCCc1ccccc1OC(=O)c1ccccc1Br
Mol. weight [g/mol]: 319.19

Physical Properties

Property code	Value	Unit	Source
gf	69.80	kJ/mol	Joback Method
hf	-141.92	kJ/mol	Joback Method
hfus	32.57	kJ/mol	Joback Method
hvap	72.68	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	4.621		Crippen Method
mcvol	213.720	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
rinpol	2199.00		NIST Webbook
rinpol	2199.00		NIST Webbook
tb	771.25	K	Joback Method
tc	1015.67	K	Joback Method
tf	479.92	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.92	J/mol×K	771.25	Joback Method
cpg	567.88	J/mol×K	811.99	Joback Method
cpg	580.69	J/mol×K	852.72	Joback Method
cpg	592.39	J/mol×K	893.46	Joback Method
cpg	603.05	J/mol×K	934.20	Joback Method
cpg	612.74	J/mol×K	974.93	Joback Method
cpg	621.51	J/mol×K	1015.67	Joback Method
dvisc	0.0007298	Pa×s	479.92	Joback Method

dvisc	0.0004579	Pa×s	528.48	Joback Method
dvisc	0.0003108	Pa×s	577.03	Joback Method
dvisc	0.0002240	Pa×s	625.59	Joback Method
dvisc	0.0001693	Pa×s	674.14	Joback Method
dvisc	0.0001328	Pa×s	722.69	Joback Method
dvisc	0.0001074	Pa×s	771.25	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U354675&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