3-Bromobenzoic acid, 3-methylphenyl ester

Inchi: InChI=1S/C14H11BrO2/c1-10-4-2-7-13(8-10)17-14(16)11-5-3-6-12(15)9-11/h2-9H,1H3
InchiKey: NMQQMNGWYHVNLO-UHFFFAOYSA-N
Formula: C14H11BrO2
SMILES: Cc1cccc(OC(=O)c2cccc(Br)c2)c1
Mol. weight [g/mol]: 291.14

Physical Properties

Property code	Value	Unit	Source
gf	52.96	kJ/mol	Joback Method
hf	-100.64	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	68.22	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.977		Crippen Method
mcvol	185.540	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	2008.00		NIST Webbook
rinpol	2008.00		NIST Webbook
tb	725.49	K	Joback Method
tc	980.66	K	Joback Method
tf	457.38	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.93	J/mol×K	725.49	Joback Method
cpg	503.71	J/mol×K	938.13	Joback Method
cpg	494.80	J/mol×K	895.60	Joback Method
cpg	484.93	J/mol×K	853.07	Joback Method
cpg	474.03	J/mol×K	810.55	Joback Method
cpg	462.05	J/mol×K	768.02	Joback Method
cpg	511.71	J/mol×K	980.66	Joback Method
dvisc	0.0001373	Pa×s	725.49	Joback Method

dvisc	0.0001683	Pa×s	680.81	Joback Method
dvisc	0.0002121	Pa×s	636.12	Joback Method
dvisc	0.0002770	Pa×s	591.43	Joback Method
dvisc	0.0003778	Pa×s	546.75	Joback Method
dvisc	0.0005446	Pa×s	502.06	Joback Method
dvisc	0.0008431	Pa×s	457.38	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=U307548&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