3-Bromobenzoic acid, 2-chlorophenyl ester

Inchi: InChI=1S/C13H8BrClO2/c14-10-5-3-4-9(8-10)13(16)17-12-7-2-1-6-11(12)15/h1-8H
InchiKey: GLMMOSUCBIPMQS-UHFFFAOYSA-N
Formula: C13H8BrClO2
SMILES: O=C(Oc1ccccc1Cl)c1cccc(Br)c1
Mol. weight [g/mol]: 311.56

Physical Properties

Property code	Value	Unit	Source
gf	32.61	kJ/mol	Joback Method
hf	-95.74	kJ/mol	Joback Method
hfus	29.00	kJ/mol	Joback Method
hvap	70.38	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.322		Crippen Method
mcvol	183.690	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	2107.50		NIST Webbook
tb	740.04	K	Joback Method
tc	1003.05	K	Joback Method
tf	476.03	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.51	J/mol×K	740.04	Joback Method
cpg	465.68	J/mol×K	959.22	Joback Method
cpg	458.37	J/mol×K	915.38	Joback Method
cpg	450.16	J/mol×K	871.55	Joback Method
cpg	440.98	J/mol×K	827.71	Joback Method
cpg	430.79	J/mol×K	783.88	Joback Method
cpg	472.17	J/mol×K	1003.05	Joback Method
dvisc	0.0001396	Pa×s	740.04	Joback Method
dvisc	0.0001702	Pa×s	696.04	Joback Method

dvisc	0.0002132	Pa×s	652.04	Joback Method
dvisc	0.0002759	Pa×s	608.03	Joback Method
dvisc	0.0003717	Pa×s	564.03	Joback Method
dvisc	0.0005267	Pa×s	520.03	Joback Method
dvisc	0.0007959	Pa×s	476.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292665&Units=SI
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

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