3-Bromobenzoic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C13H7BrCl2O2/c14-9-3-1-2-8(6-9)13(17)18-10-4-5-11(15)12(16)7-10/h1-7H
InchiKey: PHBPGBKWKJBKOG-UHFFFAOYSA-N
Formula: C13H7BrCl2O2
SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)c1cccc(Br)c1
Mol. weight [g/mol]: 346.00

Physical Properties

Property code	Value	Unit	Source
gf	11.05	kJ/mol	Joback Method
hf	-122.95	kJ/mol	Joback Method
hfus	32.81	kJ/mol	Joback Method
hvap	75.43	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	4.975		Crippen Method
mcvol	195.930	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	2304.00		NIST Webbook
rinpol	2304.00		NIST Webbook
tb	782.45	K	Joback Method
tc	1047.67	K	Joback Method
tf	518.47	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.33	J/mol×K	782.45	Joback Method
cpg	447.27	J/mol×K	826.65	Joback Method
cpg	456.19	J/mol×K	870.86	Joback Method
cpg	464.15	J/mol×K	915.06	Joback Method
cpg	471.21	J/mol×K	959.26	Joback Method
cpg	477.43	J/mol×K	1003.47	Joback Method
cpg	482.86	J/mol×K	1047.67	Joback Method
dvisc	0.0006118	Pa×s	518.47	Joback Method

dvisc	0.0004232	Pa×s	562.47	Joback Method
dvisc	0.0003088	Pa×s	606.46	Joback Method
dvisc	0.0002351	Pa×s	650.46	Joback Method
dvisc	0.0001853	Pa×s	694.46	Joback Method
dvisc	0.0001503	Pa×s	738.45	Joback Method
dvisc	0.0001248	Pa×s	782.45	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=U307553&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