4-Bromobenzoic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C13H5BrCl4O2/c14-7-3-1-6(2-4-7)13(19)20-12-9(16)5-8(15)10(17)11(12)18/h1

InchiKey: XVVROJFYSIDWLV-UHFFFAOYSA-N

Formula: C13H5BrCl4O2

SMILES: O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)c1ccc(Br)cc1

Mol. weight [g/mol]: 414.89

Physical Properties

Property code	Value	Unit	Source
gf	-32.07	kJ/mol	Joback Method
hf	-177.37	kJ/mol	Joback Method
hfus	40.42	kJ/mol	Joback Method
hvap	85.52	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.282		Crippen Method
mcvol	220.410	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook
tb	867.27	K	Joback Method
tc	1136.20	K	Joback Method
tf	603.35	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.89	J/mol×K	867.27	Joback Method
cpg	475.36	J/mol×K	912.09	Joback Method
cpg	481.93	J/mol×K	956.91	Joback Method
cpg	487.64	J/mol×K	1001.74	Joback Method
cpg	492.52	J/mol×K	1046.56	Joback Method
cpg	496.62	J/mol×K	1091.38	Joback Method
cpg	499.98	J/mol×K	1136.20	Joback Method
dvisc	0.0003773	Pa×s	603.35	Joback Method

dvisc	0.0002789	Pa×s	647.34	Joback Method
dvisc	0.0002142	Pa×s	691.32	Joback Method
dvisc	0.0001698	Pa×s	735.31	Joback Method
dvisc	0.0001382	Pa×s	779.30	Joback Method
dvisc	0.0001150	Pa×s	823.28	Joback Method
dvisc	0.0000975	Pa×s	867.27	Joback Method

Sources

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=U354622&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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