

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

Inchi:	InChI=1S/C13H5BrCl4O2/c14-7-3-1-2-6(4-7)13(19)20-12-9(16)5-8(15)10(17)11(12)18/h1
InchiKey:	JQIJQJVEBHQHCH-UHFFFAOYSA-N
Formula:	C13H5BrCl4O2
SMILES:	O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)c1cccc(Br)c1
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
mvol	220.410	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	2663.00		NIST Webbook
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tb	867.27	K	Joback Method
tc	1136.20	K	Joback Method
tf	603.35	K	Joback Method
vc	0.830	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.89	J/molxK	867.27	Joback Method
cpg	496.62	J/molxK	1091.38	Joback Method
cpg	492.52	J/molxK	1046.56	Joback Method
cpg	487.64	J/molxK	1001.74	Joback Method
cpg	481.93	J/molxK	956.91	Joback Method
cpg	475.36	J/molxK	912.09	Joback Method
cpg	499.98	J/molxK	1136.20	Joback Method
dvisc	0.0000975	Paxs	867.27	Joback Method

dvisc	0.0001150	Paxs	823.28	Joback Method
dvisc	0.0001382	Paxs	779.30	Joback Method
dvisc	0.0001698	Paxs	735.31	Joback Method
dvisc	0.0002142	Paxs	691.32	Joback Method
dvisc	0.0002789	Paxs	647.34	Joback Method
dvisc	0.0003773	Paxs	603.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355189&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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