

# 4-Bromobenzoic acid, 2,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C13H6BrCl3O2/c14-8-3-1-7(2-4-8)13(18)19-12-6-10(16)9(15)5-11(12)17/h1-6H
InchiKey:	SPLGREMAUYPNISI-UHFFFAOYSA-N
Formula:	C13H6BrCl3O2
SMILES:	O=C(Oc1cc(Cl)c(Cl)cc1Cl)c1ccc(Br)cc1
Mol. weight [g/mol]:	380.45

## Physical Properties

Property code	Value	Unit	Source
gf	-10.51	kJ/mol	Joback Method
hf	-150.16	kJ/mol	Joback Method
hfus	36.62	kJ/mol	Joback Method
hvap	80.48	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	5.629		Crippen Method
mcvol	208.170	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	2533.00		NIST Webbook
rinpol	2533.00		NIST Webbook
tb	824.86	K	Joback Method
tc	1092.02	K	Joback Method
tf	560.91	K	Joback Method
vc	0.780	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.41	J/molxK	824.86	Joback Method
cpg	462.08	J/molxK	869.39	Joback Method
cpg	469.80	J/molxK	913.91	Joback Method
cpg	476.61	J/molxK	958.44	Joback Method
cpg	482.57	J/molxK	1002.97	Joback Method
cpg	487.72	J/molxK	1047.49	Joback Method
cpg	492.12	J/molxK	1092.02	Joback Method
dvisc	0.0004776	Paxs	560.91	Joback Method

dvisc	0.0003426	Paxs	604.90	Joback Method
dvisc	0.0002570	Paxs	648.89	Joback Method
dvisc	0.0002000	Paxs	692.88	Joback Method
dvisc	0.0001604	Paxs	736.88	Joback Method
dvisc	0.0001318	Paxs	780.87	Joback Method
dvisc	0.0001107	Paxs	824.86	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U354621&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354621&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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