

# p-Toluic acid, 2-bromo-4-fluorophenyl ester

<b>Other names:</b>	p-Toluylic acid, 2-bromo-4-fluorophenyl ester
<b>Inchi:</b>	InChI=1S/C14H10BrFO2/c1-9-2-4-10(5-3-9)14(17)18-13-7-6-11(16)8-12(13)15/h2-8H,1H
<b>InchiKey:</b>	YSMOUTIJYJDMQH-UHFFFAOYSA-N
<b>Formula:</b>	C14H10BrFO2
<b>SMILES:</b>	<chem>Cc1ccc(C(=O)Oc2ccc(F)cc2Br)cc1</chem>
<b>Mol. weight [g/mol]:</b>	309.13

## Physical Properties

Property code	Value	Unit	Source
gf	-151.48	kJ/mol	Joback Method
hf	-308.22	kJ/mol	Joback Method
hfus	30.08	kJ/mol	Joback Method
hvap	68.07	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.116		Crippen Method
mcvol	187.310	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
rinpol	1907.40		NIST Webbook
rinpol	1907.40		NIST Webbook
tb	729.74	K	Joback Method
tc	974.22	K	Joback Method
tf	470.49	K	Joback Method
vc	0.708	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.34	J/molxK	729.74	Joback Method
cpg	467.65	J/molxK	770.49	Joback Method
cpg	478.93	J/molxK	811.23	Joback Method
cpg	489.23	J/molxK	851.98	Joback Method
cpg	498.60	J/molxK	892.73	Joback Method
cpg	507.07	J/molxK	933.47	Joback Method
cpg	514.69	J/molxK	974.22	Joback Method

# Sources

<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=U292644&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292644&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>rinpola:</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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