

# 4-Bromobenzoic acid, 3,5-difluorophenyl ester

<b>Inchi:</b>	InChI=1S/C13H7BrF2O2/c14-9-3-1-8(2-4-9)13(17)18-12-6-10(15)5-11(16)7-12/h1-7H
<b>InchiKey:</b>	AKSUSAVQAWZIEF-UHFFFAOYSA-N
<b>Formula:</b>	C13H7BrF2O2
<b>SMILES:</b>	O=C(Oc1cc(F)cc(F)c1)c1ccc(Br)cc1
<b>Mol. weight [g/mol]:</b>	313.09

## Physical Properties

Property code	Value	Unit	Source
gf	-354.71	kJ/mol	Joback Method
hf	-483.69	kJ/mol	Joback Method
hfus	30.57	kJ/mol	Joback Method
hvap	65.03	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	3.947		Crippen Method
mvol	174.990	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1817.00		NIST Webbook
rinpol	1817.00		NIST Webbook
tb	706.13	K	Joback Method
tc	944.68	K	Joback Method
tf	459.81	K	Joback Method
vc	0.669	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.69	J/molxK	706.13	Joback Method
cpg	423.80	J/molxK	745.89	Joback Method
cpg	433.98	J/molxK	785.65	Joback Method
cpg	443.28	J/molxK	825.41	Joback Method
cpg	451.73	J/molxK	865.16	Joback Method
cpg	459.37	J/molxK	904.92	Joback Method
cpg	466.23	J/molxK	944.68	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=U299025&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299025&amp;Units=SI</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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