

# Succinic acid, 3-methylbut-2-yl 2-bromo-4-fluorophenyl ester

**Inchi:** InChI=1S/C15H18BrFO4/c1-9(2)10(3)20-14(18)6-7-15(19)21-13-5-4-11(17)8-12(13)16/h  
**InchiKey:** NNBITSKAHLQOED-UHFFFAOYSA-N  
**Formula:** C15H18BrFO4  
**SMILES:** CC(C)C(C)OC(=O)CCC(=O)Oc1ccc(F)cc1Br  
**Mol. weight [g/mol]:** 361.20

## Physical Properties

Property code	Value	Unit	Source
gf	-484.64	kJ/mol	Joback Method
hf	-809.28	kJ/mol	Joback Method
hfus	34.76	kJ/mol	Joback Method
hvap	75.74	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.861		Crippen Method
mvol	232.600	ml/mol	McGowan Method
pc	2019.95	kPa	Joback Method
rinpol	2057.00		NIST Webbook
rinpol	2057.00		NIST Webbook
tb	796.37	K	Joback Method
tc	1009.92	K	Joback Method
tf	484.98	K	Joback Method
vc	0.883	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.72	J/mol×K	796.37	Joback Method
cpg	652.69	J/mol×K	831.96	Joback Method
cpg	664.67	J/mol×K	867.55	Joback Method
cpg	675.68	J/mol×K	903.14	Joback Method
cpg	685.74	J/mol×K	938.74	Joback Method
cpg	694.85	J/mol×K	974.33	Joback Method
cpg	703.03	J/mol×K	1009.92	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=U389764&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U389764&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>h vap:</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>r in pol:</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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