

# Succinic acid, naphth-2-ylmethyl 2-bromo-4-fluorophenyl ester

<b>Inchi:</b>	InChI=1S/C21H16BrFO4/c22-18-12-17(23)7-8-19(18)27-21(25)10-9-20(24)26-13-14-5-6
<b>InchiKey:</b>	VQAZQCUJTDLJDX-UHFFFAOYSA-N
<b>Formula:</b>	C21H16BrFO4
<b>SMILES:</b>	O=C(CCC(=O)Oc1ccc(F)cc1Br)OCc1ccc2ccccc2c1
<b>Mol. weight [g/mol]:</b>	431.25

## Physical Properties

Property code	Value	Unit	Source
gf	-219.81	kJ/mol	Joback Method
hf	-506.43	kJ/mol	Joback Method
hfus	48.02	kJ/mol	Joback Method
hvap	94.45	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	5.170		Crippen Method
mcvol	273.920	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinsol	3193.00		NIST Webbook
tb	985.17	K	Joback Method
tc	1229.26	K	Joback Method
tf	654.24	K	Joback Method
vc	1.046	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.02	J/mol×K	985.17	Joback Method
cpg	803.49	J/mol×K	1025.85	Joback Method
cpg	812.95	J/mol×K	1066.53	Joback Method
cpg	821.49	J/mol×K	1107.22	Joback Method
cpg	829.19	J/mol×K	1147.90	Joback Method
cpg	836.13	J/mol×K	1188.58	Joback Method
cpg	842.40	J/mol×K	1229.26	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=U389778&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U389778&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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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