

# Dimethylmalonic acid, 2-bromo-4-fluorophenyl heptyl ester

<b>Inchi:</b>	InChI=1S/C18H24BrFO4/c1-4-5-6-7-8-11-23-16(21)18(2,3)17(22)24-15-10-9-13(20)12-14
<b>InchiKey:</b>	GZPYYKMILXYCAZ-UHFFFAOYSA-N
<b>Formula:</b>	C18H24BrFO4
<b>SMILES:</b>	CCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccc(F)cc1Br
<b>Mol. weight [g/mol]:</b>	403.28

## Physical Properties

Property code	Value	Unit	Source
gf	-451.66	kJ/mol	Joback Method
hf	-869.39	kJ/mol	Joback Method
hfus	42.16	kJ/mol	Joback Method
hvap	81.90	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.033		Crippen Method
mvol	274.870	ml/mol	McGowan Method
pc	1587.28	kPa	Joback Method
rinpol	2199.00		NIST Webbook
rinpol	2199.00		NIST Webbook
tb	862.66	K	Joback Method
tc	1074.64	K	Joback Method
tf	551.21	K	Joback Method
vc	1.052	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.63	J/mol×K	862.66	Joback Method
cpg	822.27	J/mol×K	897.99	Joback Method
cpg	834.88	J/mol×K	933.32	Joback Method
cpg	846.50	J/mol×K	968.65	Joback Method
cpg	857.16	J/mol×K	1003.98	Joback Method
cpg	866.92	J/mol×K	1039.31	Joback Method
cpg	875.82	J/mol×K	1074.64	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U361824&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361824&amp;Units=SI</a>
<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.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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>hvp:</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>rinp:</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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