

# Fumaric acid, 4-bromophenyl 2-ethylhexyl ester

Inchi:	InChI=1S/C18H23BrO4/c1-3-5-6-14(4-2)13-22-17(20)11-12-18(21)23-16-9-7-15(19)8-10
InchiKey:	UEDJPDQMTDLZMH-VAWYXSNFSA-N
Formula:	C18H23BrO4
SMILES:	CCCCC(CC)COC(=O)C=CC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]:	383.28

## Physical Properties

Property code	Value	Unit	Source
gf	-172.28	kJ/mol	Joback Method
hf	-541.12	kJ/mol	Joback Method
hfus	43.57	kJ/mol	Joback Method
hvap	82.92	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.670		Crippen Method
mcvol	268.800	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	2507.00		NIST Webbook
rinpol	2507.00		NIST Webbook
tb	865.36	K	Joback Method
tc	1083.00	K	Joback Method
tf	515.60	K	Joback Method
vc	1.020	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.63	J/molxK	865.36	Joback Method
cpg	788.35	J/molxK	901.63	Joback Method
cpg	801.03	J/molxK	937.91	Joback Method
cpg	812.72	J/molxK	974.18	Joback Method
cpg	823.47	J/molxK	1010.46	Joback Method
cpg	833.31	J/molxK	1046.73	Joback Method
cpg	842.29	J/molxK	1083.00	Joback Method
dvisc	0.0004933	Paxs	515.60	Joback Method

dvisc	0.0002719	Paxs	573.89	Joback Method
dvisc	0.0001673	Paxs	632.19	Joback Method
dvisc	0.0001117	Paxs	690.48	Joback Method
dvisc	0.0000795	Paxs	748.77	Joback Method
dvisc	0.0000594	Paxs	807.07	Joback Method
dvisc	0.0000461	Paxs	865.36	Joback Method

## Sources

<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=U405772&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405772&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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>rinpol:</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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