

# Fumaric acid, 2-octyl 2,3-dichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C18H22Cl2O4/c1-3-4-5-6-8-13(2)23-16(21)11-12-17(22)24-15-10-7-9-14(19)18
<b>InchiKey:</b>	BOPSOZYKDHLOCW-VAWYXSNFSA-N
<b>Formula:</b>	C18H22Cl2O4
<b>SMILES:</b>	CCCCCCC(C)OC(=O)C=CC(=O)Oc1cccc(Cl)c1Cl
<b>Mol. weight [g/mol]:</b>	373.27

## Physical Properties

Property code	Value	Unit	Source
gf	-220.09	kJ/mol	Joback Method
hf	-610.40	kJ/mol	Joback Method
hfus	46.29	kJ/mol	Joback Method
hvap	85.91	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.357		Crippen Method
mcvol	275.780	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	2530.00		NIST Webbook
rinpol	2530.00		NIST Webbook
tb	879.04	K	Joback Method
tc	1095.34	K	Joback Method
tf	528.16	K	Joback Method
vc	1.056	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.49	J/molxK	879.04	Joback Method
cpg	840.15	J/molxK	1059.29	Joback Method
cpg	831.18	J/molxK	1023.24	Joback Method
cpg	821.26	J/molxK	987.19	Joback Method
cpg	810.36	J/molxK	951.14	Joback Method
cpg	798.45	J/molxK	915.09	Joback Method
cpg	848.20	J/molxK	1095.34	Joback Method
dvisc	0.0000439	Paxs	879.04	Joback Method

dvisc	0.0000561	Paxs	820.56	Joback Method
dvisc	0.0000745	Paxs	762.08	Joback Method
dvisc	0.0001037	Paxs	703.60	Joback Method
dvisc	0.0001532	Paxs	645.12	Joback Method
dvisc	0.0002447	Paxs	586.64	Joback Method
dvisc	0.0004334	Paxs	528.16	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=U405591&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405591&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.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>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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