

# Fumaric acid, 3,5-dichlorophenyl isoheptyl ester

<b>Inchi:</b>	InChI=1S/C16H18Cl2O4/c1-11(2)4-3-7-21-15(19)5-6-16(20)22-14-9-12(17)8-13(18)10-14
<b>InchiKey:</b>	OHLCSBOWTPMGNR-AATRIKPKSA-N
<b>Formula:</b>	C16H18Cl2O4
<b>SMILES:</b>	CC(C)CCCOC(=O)C=CC(=O)Oc1cc(Cl)cc(Cl)c1
<b>Mol. weight [g/mol]:</b>	345.22

## Physical Properties

Property code	Value	Unit	Source
gf	-236.93	kJ/mol	Joback Method
hf	-569.12	kJ/mol	Joback Method
hfus	41.11	kJ/mol	Joback Method
hvap	81.46	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.434		Crippen Method
mvol	247.600	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	2378.00		NIST Webbook
rinpol	2378.00		NIST Webbook
tb	833.28	K	Joback Method
tc	1052.04	K	Joback Method
tf	505.62	K	Joback Method
vc	0.944	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.75	J/molxK	833.28	Joback Method
cpg	685.18	J/molxK	869.74	Joback Method
cpg	696.62	J/molxK	906.20	Joback Method
cpg	707.11	J/molxK	942.66	Joback Method
cpg	716.66	J/molxK	979.12	Joback Method
cpg	725.30	J/molxK	1015.58	Joback Method
cpg	733.05	J/molxK	1052.04	Joback Method
dvisc	0.0005311	Paxs	505.62	Joback Method

dvisc	0.0003071	Paxs	560.23	Joback Method
dvisc	0.0001957	Paxs	614.84	Joback Method
dvisc	0.0001343	Paxs	669.45	Joback Method
dvisc	0.0000975	Paxs	724.06	Joback Method
dvisc	0.0000740	Paxs	778.67	Joback Method
dvisc	0.0000583	Paxs	833.28	Joback Method

## Sources

<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=U348236&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348236&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>

## 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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