

# Fumaric acid, isoheptyl 2,3,5-trichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C16H17Cl3O4/c1-10(2)4-3-7-22-14(20)5-6-15(21)23-13-9-11(17)8-12(18)16(19)
<b>InchiKey:</b>	ZJEUAPZXNZRZAM-AATRIKPKSA-N
<b>Formula:</b>	C16H17Cl3O4
<b>SMILES:</b>	CC(C)CCCOC(=O)C=CC(=O)Oc1cc(Cl)cc(Cl)c1Cl
<b>Mol. weight [g/mol]:</b>	379.66

## Physical Properties

Property code	Value	Unit	Source
gf	-258.49	kJ/mol	Joback Method
hf	-596.33	kJ/mol	Joback Method
hfus	44.91	kJ/mol	Joback Method
hvap	86.51	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.088		Crippen Method
mcvol	259.840	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinsol	2488.00		NIST Webbook
tb	875.69	K	Joback Method
tc	1098.72	K	Joback Method
tf	548.06	K	Joback Method
vc	0.993	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.24	J/molxK	875.69	Joback Method
cpg	739.72	J/molxK	1061.55	Joback Method
cpg	732.30	J/molxK	1024.38	Joback Method
cpg	723.97	J/molxK	987.20	Joback Method
cpg	714.70	J/molxK	950.03	Joback Method
cpg	704.46	J/molxK	912.86	Joback Method
cpg	746.25	J/molxK	1098.72	Joback Method
dvisc	0.0000510	Paxs	875.69	Joback Method
dvisc	0.0000639	Paxs	821.09	Joback Method

dvisc	0.0000826	Paxs	766.48	Joback Method
dvisc	0.0001111	Paxs	711.88	Joback Method
dvisc	0.0001570	Paxs	657.27	Joback Method
dvisc	0.0002361	Paxs	602.67	Joback Method
dvisc	0.0003853	Paxs	548.06	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U348144&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348144&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>
<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>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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