

# Adipic acid, 2,2-dichloroethyl heptyl ester

<b>Inchi:</b>	InChI=1S/C15H26Cl2O4/c1-2-3-4-5-8-11-20-14(18)9-6-7-10-15(19)21-12-13(16)17/h13H
<b>InchiKey:</b>	ZOPNTMOQCRBBSX-UHFFFAOYSA-N
<b>Formula:</b>	C15H26Cl2O4
<b>SMILES:</b>	CCCCCCCOC(=O)CCCCC(=O)OCC(Cl)Cl
<b>Mol. weight [g/mol]:</b>	341.27

## Physical Properties

Property code	Value	Unit	Source
gf	-418.72	kJ/mol	Joback Method
hf	-879.29	kJ/mol	Joback Method
hfus	45.05	kJ/mol	Joback Method
hvap	75.68	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.407		Crippen Method
mvol	261.570	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
rinpol	2194.00		NIST Webbook
rinpol	2194.00		NIST Webbook
tb	769.60	K	Joback Method
tc	957.30	K	Joback Method
tf	447.97	K	Joback Method
vc	1.016	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.73	J/molxK	769.60	Joback Method
cpg	802.08	J/molxK	926.02	Joback Method
cpg	790.89	J/molxK	894.74	Joback Method
cpg	778.87	J/molxK	863.45	Joback Method
cpg	766.01	J/molxK	832.17	Joback Method
cpg	752.30	J/molxK	800.88	Joback Method
cpg	812.46	J/molxK	957.30	Joback Method
dvisc	0.0000748	Paxs	769.60	Joback Method

dvisc	0.0000986	Paxs	715.99	Joback Method
dvisc	0.0001360	Paxs	662.39	Joback Method
dvisc	0.0001983	Paxs	608.78	Joback Method
dvisc	0.0003112	Paxs	555.18	Joback Method
dvisc	0.0005376	Paxs	501.57	Joback Method
dvisc	0.0010585	Paxs	447.97	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=U353581&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353581&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>

## 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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