

# 1,2-Cyclohexanedicarboxylic acid, 2,5-dichlorophenyl hexyl ester

Inchi:	InChI=1S/C20H26Cl2O4/c1-2-3-4-7-12-25-19(23)15-8-5-6-9-16(15)20(24)26-18-13-14(2
InchiKey:	QSNsoJBPjBXNTE-UHFFFAOYSA-N
Formula:	C20H26Cl2O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	401.32

## Physical Properties

Property code	Value	Unit	Source
gf	-264.29	kJ/mol	Joback Method
hf	-729.64	kJ/mol	Joback Method
hfus	47.69	kJ/mol	Joback Method
hvap	90.92	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.829		Crippen Method
mcvol	297.400	ml/mol	McGowan Method
pc	1427.22	kPa	Joback Method
rinpol	2727.00		NIST Webbook
rinpol	2727.00		NIST Webbook
tb	935.96	K	Joback Method
tc	1163.56	K	Joback Method
tf	573.92	K	Joback Method
vc	1.125	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	927.19	J/molxK	935.96	Joback Method
cpg	941.16	J/molxK	973.89	Joback Method
cpg	953.55	J/molxK	1011.83	Joback Method
cpg	964.37	J/molxK	1049.76	Joback Method
cpg	973.66	J/molxK	1087.69	Joback Method
cpg	981.43	J/molxK	1125.62	Joback Method
cpg	987.71	J/molxK	1163.56	Joback Method
dvisc	0.0004465	Paxs	573.92	Joback Method

dvisc	0.0002680	Paxs	634.26	Joback Method
dvisc	0.0001757	Paxs	694.60	Joback Method
dvisc	0.0001233	Paxs	754.94	Joback Method
dvisc	0.0000912	Paxs	815.28	Joback Method
dvisc	0.0000703	Paxs	875.62	Joback Method
dvisc	0.0000560	Paxs	935.96	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U339801&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339801&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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