

# 2,2-dichloroethyl heptanoate

**Inchi:** InChI=1S/C9H16Cl2O2/c1-2-3-4-5-6-9(12)13-7-8(10)11/h8H,2-7H2,1H3  
**InchiKey:** KKDZZVNLJUMCED-UHFFFAOYSA-N  
**Formula:** C9H16Cl2O2  
**SMILES:** CCCCCC(=O)OCC(Cl)Cl  
**Mol. weight [g/mol]:** 227.13

## Physical Properties

Property code	Value	Unit	Source
gf	-235.32	kJ/mol	Joback Method
hf	-510.65	kJ/mol	Joback Method
hfus	26.72	kJ/mol	Joback Method
hvap	53.17	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.304		Crippen Method
mcvol	169.590	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
ripol	1378.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1378.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1900.00		NIST Webbook
ripol	1860.00		NIST Webbook
ripol	1900.00		NIST Webbook
ripol	1854.00		NIST Webbook
ripol	1886.00		NIST Webbook
ripol	1852.00		NIST Webbook
ripol	1869.00		NIST Webbook
ripol	1850.00		NIST Webbook
ripol	1850.00		NIST Webbook
tb	556.03	K	Joback Method
tc	743.61	K	Joback Method
tf	308.19	K	Joback Method
vc	0.655	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.33	J/molxK	556.03	Joback Method
cpg	437.41	J/molxK	712.35	Joback Method
cpg	427.10	J/molxK	681.08	Joback Method
cpg	416.25	J/molxK	649.82	Joback Method
cpg	404.84	J/molxK	618.56	Joback Method
cpg	392.87	J/molxK	587.29	Joback Method
cpg	447.18	J/molxK	743.61	Joback Method
dvisc	0.0002166	Paxs	556.03	Joback Method
dvisc	0.0002852	Paxs	514.72	Joback Method
dvisc	0.0003940	Paxs	473.42	Joback Method
dvisc	0.0005790	Paxs	432.11	Joback Method
dvisc	0.0009231	Paxs	390.80	Joback Method
dvisc	0.0016431	Paxs	349.50	Joback Method
dvisc	0.0034137	Paxs	308.19	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R30620&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R30620&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>

## 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>ripol:</b>	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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