

# Diethylmalonic acid, butyl 2,2-dichloroethyl ester

Inchi:	InChI=1S/C13H22Cl2O4/c1-4-7-8-18-11(16)13(5-2,6-3)12(17)19-9-10(14)15/h10H,4-9H2
InchiKey:	UIKNEZQCNJTCFT-UHFFFAOYSA-N
Formula:	C13H22Cl2O4
SMILES:	CCCCOC(=O)C(CC)(CC)C(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	313.22

## Physical Properties

Property code	Value	Unit	Source
gf	-432.72	kJ/mol	Joback Method
hf	-846.76	kJ/mol	Joback Method
hfus	32.46	kJ/mol	Joback Method
hvap	69.93	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.483		Crippen Method
mcvol	233.390	ml/mol	McGowan Method
pc	1706.12	kPa	Joback Method
rinpol	1708.00		NIST Webbook
rinpol	1708.00		NIST Webbook
tb	720.61	K	Joback Method
tc	915.82	K	Joback Method
tf	427.85	K	Joback Method
vc	0.892	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.55	J/molxK	720.61	Joback Method
cpg	643.55	J/molxK	753.15	Joback Method
cpg	656.70	J/molxK	785.68	Joback Method
cpg	669.02	J/molxK	818.22	Joback Method
cpg	680.53	J/molxK	850.75	Joback Method
cpg	691.26	J/molxK	883.29	Joback Method
cpg	701.22	J/molxK	915.82	Joback Method
dvisc	0.0012908	Paxs	427.85	Joback Method

dvisc	0.0006461	Paxs	476.64	Joback Method
dvisc	0.0003678	Paxs	525.44	Joback Method
dvisc	0.0002304	Paxs	574.23	Joback Method
dvisc	0.0001553	Paxs	623.02	Joback Method
dvisc	0.0001109	Paxs	671.82	Joback Method
dvisc	0.0000828	Paxs	720.61	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=U370779&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370779&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>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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