

# Diethylmalonic acid, 3-phenoxybenzyl propyl ester

Inchi:	InChI=1S/C23H28O5/c1-4-15-26-21(24)23(5-2,6-3)22(25)27-17-18-11-10-14-20(16-18)2
InchiKey:	QZLIUKIMWKFFFQ-UHFFFAOYSA-N
Formula:	C23H28O5
SMILES:	CCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]:	384.47

## Physical Properties

Property code	Value	Unit	Source
gf	-212.03	kJ/mol	Joback Method
hf	-687.03	kJ/mol	Joback Method
hfus	42.37	kJ/mol	Joback Method
hvap	91.43	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.282		Crippen Method
mcvol	308.160	ml/mol	McGowan Method
pc	1387.11	kPa	Joback Method
rinsol	2626.00		NIST Webbook
tb	955.75	K	Joback Method
tc	1183.43	K	Joback Method
tf	583.30	K	Joback Method
vc	1.163	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	984.93	J/molxK	955.75	Joback Method
cpg	1040.11	J/molxK	1145.48	Joback Method
cpg	1031.68	J/molxK	1107.54	Joback Method
cpg	1022.01	J/molxK	1069.59	Joback Method
cpg	1011.03	J/molxK	1031.64	Joback Method
cpg	998.69	J/molxK	993.70	Joback Method
cpg	1047.35	J/molxK	1183.43	Joback Method
dvisc	0.0000209	Paxs	955.75	Joback Method
dvisc	0.0000271	Paxs	893.67	Joback Method

dvisc	0.0000365	Paxs	831.60	Joback Method
dvisc	0.0000518	Paxs	769.53	Joback Method
dvisc	0.0000780	Paxs	707.45	Joback Method
dvisc	0.0001270	Paxs	645.38	Joback Method
dvisc	0.0002296	Paxs	583.30	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=U370230&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370230&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>

## 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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