

# Pimelic acid, dodecyl 2-(2-methoxyethyl)heptyl ester

Inchi:	InChI=1S/C29H56O5/c1-4-6-8-9-10-11-12-13-14-19-24-33-28(30)21-17-15-18-22-29(31)
InchiKey:	QLPNCNXQTYRXDP-UHFFFAOYSA-N
Formula:	C29H56O5
SMILES:	CCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(CCCCC)CCOC
Mol. weight [g/mol]:	484.75

## Physical Properties

Property code	Value	Unit	Source
gf	-381.98	kJ/mol	Joback Method
hf	-1268.99	kJ/mol	Joback Method
hfus	74.10	kJ/mol	Joback Method
hvap	100.48	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	8.177		Crippen Method
mvol	440.220	ml/mol	McGowan Method
pc	651.10	kPa	Joback Method
rinpol	3232.00		NIST Webbook
rinpol	3232.00		NIST Webbook
tb	1037.48	K	Joback Method
tc	1300.17	K	Joback Method
tf	568.14	K	Joback Method
vc	1.720	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1570.96	J/molxK	1037.48	Joback Method
cpg	1593.43	J/molxK	1081.26	Joback Method
cpg	1613.23	J/molxK	1125.04	Joback Method
cpg	1630.43	J/molxK	1168.83	Joback Method
cpg	1645.12	J/molxK	1212.61	Joback Method
cpg	1657.35	J/molxK	1256.39	Joback Method
cpg	1667.22	J/molxK	1300.17	Joback Method
dvisc	0.0002050	Paxs	568.14	Joback Method

dvisc	0.0000886	Paxs	646.36	Joback Method
dvisc	0.0000459	Paxs	724.59	Joback Method
dvisc	0.0000270	Paxs	802.81	Joback Method
dvisc	0.0000175	Paxs	881.03	Joback Method
dvisc	0.0000121	Paxs	959.26	Joback Method
dvisc	0.0000089	Paxs	1037.48	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406740&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406740&amp;Units=SI</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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