

# 1,3-Dioxepane, 2-pentadecyl-

<b>Inchi:</b>	InChI=1S/C20H40O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-20-21-18-15-16-19-22-20/h2
<b>InchiKey:</b>	QZZVQKZZBUCTHK-UHFFFAOYSA-N
<b>Formula:</b>	C20H40O2
<b>SMILES:</b>	CCCCCCCCCCCCCCCC1OCCCCO1
<b>Mol. weight [g/mol]:</b>	312.53
<b>CAS:</b>	41563-29-5

## Physical Properties

Property code	Value	Unit	Source
gf	-42.37	kJ/mol	Joback Method
hf	-671.97	kJ/mol	Joback Method
hfus	53.25	kJ/mol	Joback Method
hvap	69.73	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.621		Crippen Method
mvol	293.540	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
tb	734.72	K	Joback Method
tc	919.11	K	Joback Method
tf	372.16	K	Joback Method
vc	1.123	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.51	J/molxK	734.72	Joback Method
cpg	944.72	J/molxK	765.45	Joback Method
cpg	965.73	J/molxK	796.18	Joback Method
cpg	985.57	J/molxK	826.91	Joback Method
cpg	1004.28	J/molxK	857.65	Joback Method
cpg	1021.88	J/molxK	888.38	Joback Method
cpg	1038.41	J/molxK	919.11	Joback Method
dvisc	0.0030626	Paxs	372.16	Joback Method
dvisc	0.0009989	Paxs	432.59	Joback Method

dvisc	0.0004288	Paxs	493.01	Joback Method
dvisc	0.0002214	Paxs	553.44	Joback Method
dvisc	0.0001302	Paxs	613.87	Joback Method
dvisc	0.0000842	Paxs	674.29	Joback Method
dvisc	0.0000585	Paxs	734.72	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=C41563295&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C41563295&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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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