

# propyl docosanoate

<b>Other names:</b>	Propyl behenate
<b>Inchi:</b>	InChI=1S/C25H50O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25(26)
<b>InchiKey:</b>	OKYLPPWXDVPDBZ-UHFFFAOYSA-N
<b>Formula:</b>	C25H50O2
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCCCCCCC(=O)OCCC
<b>Mol. weight [g/mol]:</b>	382.66
<b>CAS:</b>	26718-94-5

## Physical Properties

Property code	Value	Unit	Source
gf	-74.30	kJ/mol	Joback Method
hf	-804.13	kJ/mol	Joback Method
hfus	63.29	kJ/mol	Joback Method
hvap	80.40	kJ/mol	Joback Method
log10ws	-9.15		Crippen Method
logp	8.762		Crippen Method
mcvol	370.550	ml/mol	McGowan Method
pc	783.75	kPa	Joback Method
rinpol	2675.85		NIST Webbook
rinpol	2679.00		NIST Webbook
rinpol	2675.85		NIST Webbook
tb	847.69	K	Joback Method
tc	1038.15	K	Joback Method
tf	443.67	K	Joback Method
vc	1.460	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1220.77	J/mol×K	847.69	Joback Method
cpg	1243.05	J/mol×K	879.43	Joback Method
cpg	1264.07	J/mol×K	911.18	Joback Method
cpg	1283.89	J/mol×K	942.92	Joback Method
cpg	1302.54	J/mol×K	974.66	Joback Method

cpg	1320.07	J/molxK	1006.41	Joback Method
cpg	1336.53	J/molxK	1038.15	Joback Method
dvisc	0.0009384	Paxs	443.67	Joback Method
dvisc	0.0003813	Paxs	511.01	Joback Method
dvisc	0.0001910	Paxs	578.34	Joback Method
dvisc	0.0001106	Paxs	645.68	Joback Method
dvisc	0.0000710	Paxs	713.02	Joback Method
dvisc	0.0000492	Paxs	780.35	Joback Method
dvisc	0.0000361	Paxs	847.69	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=C26718945&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C26718945&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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