

# 2,5,8,11,14,17,20-Heptaoxadocosan-22-oic acid

**Inchi:** InChI=1S/C15H30O9/c1-18-2-3-19-4-5-20-6-7-21-8-9-22-10-11-23-12-13-24-14-15(16)17  
**InchiKey:** AWSXISOALMMMQQ-UHFFFAOYSA-N  
**Formula:** C15H30O9  
**SMILES:** COCCOCCOCCOCCOCCOCCOCC(=O)O  
**Mol. weight [g/mol]:** 354.39

## Physical Properties

Property code	Value	Unit	Source
gf	-925.32	kJ/mol	Joback Method
hf	-1543.28	kJ/mol	Joback Method
hfus	48.61	kJ/mol	Joback Method
hvap	89.28	kJ/mol	Joback Method
log10ws	1.19		Crippen Method
logp	-0.183		Crippen Method
mcvol	270.740	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
rinpol	2571.40		NIST Webbook
tb	845.59	K	Joback Method
tc	1035.30	K	Joback Method
tf	525.17	K	Joback Method
vc	1.026	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.03	J/molxK	845.59	Joback Method
cpg	931.45	J/molxK	1003.68	Joback Method
cpg	921.70	J/molxK	972.06	Joback Method
cpg	910.65	J/molxK	940.45	Joback Method
cpg	898.33	J/molxK	908.83	Joback Method
cpg	884.77	J/molxK	877.21	Joback Method
cpg	939.84	J/molxK	1035.30	Joback Method
dvisc	0.0000042	Paxs	845.59	Joback Method
dvisc	0.0000061	Paxs	792.19	Joback Method

dvisc	0.0000092	Paxs	738.78	Joback Method
dvisc	0.0000148	Paxs	685.38	Joback Method
dvisc	0.0000260	Paxs	631.98	Joback Method
dvisc	0.0000505	Paxs	578.57	Joback Method
dvisc	0.0001122	Paxs	525.17	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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=R578108&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R578108&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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