

# 2-Ethylhexyl heptadecanoate

<b>Inchi:</b>	InChI=1S/C25H50O2/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-22-25(26)27-23-24(6-
<b>InchiKey:</b>	UCSVBMVEAXFUTC-UHFFFAOYSA-N
<b>Formula:</b>	C25H50O2
<b>SMILES:</b>	CCCCCCCCCCCCCCCC(=O)OCC(CC)CCCC
<b>Mol. weight [g/mol]:</b>	382.66

## Physical Properties

Property code	Value	Unit	Source
gf	-76.74	kJ/mol	Joback Method
hf	-809.41	kJ/mol	Joback Method
hfus	59.77	kJ/mol	Joback Method
hvap	80.01	kJ/mol	Joback Method
log10ws	-8.91		Crippen Method
logp	8.617		Crippen Method
mvol	370.550	ml/mol	McGowan Method
pc	787.27	kPa	Joback Method
rinpol	2579.00		NIST Webbook
tb	847.25	K	Joback Method
tc	1037.37	K	Joback Method
tf	428.67	K	Joback Method
vc	1.454	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1221.19	J/molxK	847.25	Joback Method
cpg	1320.21	J/molxK	1005.69	Joback Method
cpg	1302.75	J/molxK	974.00	Joback Method
cpg	1284.15	J/molxK	942.31	Joback Method
cpg	1264.39	J/molxK	910.62	Joback Method
cpg	1243.42	J/molxK	878.94	Joback Method
cpg	1336.60	J/molxK	1037.37	Joback Method
dvisc	0.0000331	Paxs	847.25	Joback Method
dvisc	0.0000458	Paxs	777.49	Joback Method

dvisc	0.0000676	Paxs	707.72	Joback Method
dvisc	0.0001086	Paxs	637.96	Joback Method
dvisc	0.0001961	Paxs	568.20	Joback Method
dvisc	0.0004178	Paxs	498.43	Joback Method
dvisc	0.0011387	Paxs	428.67	Joback Method

## Sources

<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=R540371&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R540371&amp;Units=SI</a>
<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>

## 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>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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