2-Ethylhexyl stearate

InChl=1S/C26H52O2/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-21-23-26(27)28-24-25

InchiKey: OPJWPPVYCOPDCM-UHFFFAOYSA-N

Formula: C26H52O2

SMILES: CCCCCCCCCCCCCC(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 396.69 CAS: 22047-49-0

Physical Properties

Property code	Value	Unit	Source
gf	-68.32	kJ/mol	Joback Method
hf	-830.05	kJ/mol	Joback Method
hfus	62.36	kJ/mol	Joback Method
hvap	82.24	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	9.008		Crippen Method
mcvol	384.640	ml/mol	McGowan Method
рс	746.51	kPa	Joback Method
rinpol	2684.00		NIST Webbook
tb	870.13	K	Joback Method
tc	1066.30	K	Joback Method
tf	439.94	K	Joback Method
VC	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1403.60	J/mol×K	1066.30	Joback Method
cpg	1308.62	J/mol×K	902.82	Joback Method
cpg	1330.12	J/mol×K	935.52	Joback Method
cpg	1350.31	J/mol×K	968.21	Joback Method
cpg	1369.26	J/mol×K	1000.91	Joback Method
cpg	1387.01	J/mol×K	1033.60	Joback Method
cpg	1285.77	J/mol×K	870.13	Joback Method
dvisc	0.0000395	Paxs	798.43	Joback Method

dvisc	0.0000583	Paxs	726.73	Joback Method	
dvisc	0.0000940	Paxs	655.04	Joback Method	
dvisc	0.0001702	Paxs	583.34	Joback Method	
dvisc	0.0003640	Paxs	511.64	Joback Method	
dvisc	0.0000285	Paxs	870.13	Joback Method	
dvisc	0.0009974	Paxs	439.94	Joback Method	
rhol	834.40	kg/m3	328.15	Measurement and correlation of the density, viscosity and vapor pressure of fatty acid 2-ethyhexyl esters	
rhol	827.80	kg/m3	338.15	Measurement and correlation of the density, viscosity and vapor pressure of fatty acid 2-ethyhexyl esters	
rhol	824.50	kg/m3	343.15	Measurement and correlation of the density, viscosity and vapor pressure of fatty acid 2-ethyhexyl esters	
rhol	821.10	kg/m3	348.15	Measurement and correlation of the density, viscosity and vapor pressure of fatty acid 2-ethyhexyl esters	
rhol	817.20	kg/m3	353.15	Measurement and correlation of the density, viscosity and vapor pressure of fatty acid 2-ethyhexyl esters	
rhol	814.20	kg/m3	358.15	Measurement and correlation of the density, viscosity and vapor pressure of fatty acid 2-ethyhexyl esters	

rhol	811.20	kg/m3	363.15	Measurement and correlation of the density, viscosity and vapor pressure of fatty acid 2-ethyhexyl esters	
rhol	808.00	kg/m3	368.15	Measurement and correlation of the density, viscosity and vapor pressure of fatty acid 2-ethyhexyl esters	
rhol	837.70	kg/m3	323.15	Measurement and correlation of the density, viscosity and vapor pressure of fatty acid 2-ethyhexyl esters	
rhol	841.10	kg/m3	318.15	Measurement and correlation of the density, viscosity and vapor pressure of fatty acid 2-ethyhexyl esters	
rhol	844.90	kg/m3	313.15	Measurement and correlation of the density, viscosity and vapor pressure of fatty acid 2-ethyhexyl esters	
rhol	847.90	kg/m3	308.15	Measurement and correlation of the density, viscosity and vapor pressure of fatty acid 2-ethyhexyl esters	
rhol	851.40	kg/m3	303.15	Measurement and correlation of the density, viscosity and vapor pressure of fatty acid 2-ethyhexyl esters	

				the density, viscosity and vapor pressure of fatty acid 2-ethyhexyl esters	
rhol	831.10	kg/m3	333.15	Measurement and correlation of the density, viscosity and vapor pressure of fatty acid 2-ethyhexyl esters	

kg/m3

298.15

Measurement and correlation of

Sources

rhol

855.40

Measurement and correlation of the density, viscosity and vapor pressure of harry and pethylexyl esters:

https://www.doi.org/10.1016/j.jct.2018.10.012 https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:

http://webbook.nist.gov/cgi/cbook.cgi?ID=C22047490&Units=SI

Crippen Method:

http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formationhf: Enthalpy of formation at standard conditionshfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/llogp: Octanol/Water partition coefficientmcvol: McGowan's characteristic volume

pc: Critical Pressurerhol: Liquid Density

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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