

9-Octadecenoic acid (Z)-, 2-hydroxyethyl ester

Other names:	Oleic acid, 2-hydroxyethyl ester Cithrol A Ethylene glycol monooleate 2-hydroxyethyl oleate
Inchi:	InChI=1S/C20H38O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20(22)23-19-18-21/h
InchiKey:	MUHFRORXWCGZGE-KTKRTIGZSA-N
Formula:	C20H38O3
SMILES:	CCCCCCCC=CCCCCCCCC(=O)OCCO
Mol. weight [g/mol]:	326.51
CAS:	4500-01-0

Physical Properties

Property code	Value	Unit	Source
gf	-173.00	kJ/mol	Joback Method
hf	-735.94	kJ/mol	Joback Method
hfus	54.63	kJ/mol	Joback Method
hvap	85.91	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.559		Crippen Method
mcvol	301.670	ml/mol	McGowan Method
pc	1150.65	kPa	Joback Method
tb	829.63	K	Joback Method
tc	1015.86	K	Joback Method
tf	443.06	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	961.19	J/molxK	829.63	Joback Method
cpg	978.75	J/molxK	860.67	Joback Method
cpg	995.39	J/molxK	891.71	Joback Method
cpg	1011.14	J/molxK	922.74	Joback Method
cpg	1026.05	J/molxK	953.78	Joback Method

cpg	1040.14	J/mol×K	984.82	Joback Method
cpg	1053.47	J/mol×K	1015.86	Joback Method
dvisc	0.0009269	Paxs	443.06	Joback Method
dvisc	0.0002737	Paxs	507.49	Joback Method
dvisc	0.0001063	Paxs	571.92	Joback Method
dvisc	0.0000500	Paxs	636.35	Joback Method
dvisc	0.0000271	Paxs	700.77	Joback Method
dvisc	0.0000162	Paxs	765.20	Joback Method
dvisc	0.0000105	Paxs	829.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4500010&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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