

Oleic acid, 3-hydroxypropyl ester

Other names:	3-Hydroxypropyl oleate
Inchi:	InChI=1S/C21H40O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-18-21(23)24-20-17-19-22
InchiKey:	YWBLIYFXWVRDAA-KTKRTIGZSA-N
Formula:	C21H40O3
SMILES:	CCCCCCCCC=CCCCCCCCC(=O)OCCCO
Mol. weight [g/mol]:	340.54
CAS:	821-17-0

Physical Properties

Property code	Value	Unit	Source
gf	-164.58	kJ/mol	Joback Method
hf	-756.58	kJ/mol	Joback Method
hfus	57.22	kJ/mol	Joback Method
hvap	88.13	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.950		Crippen Method
mcvol	315.760	ml/mol	McGowan Method
pc	1079.22	kPa	Joback Method
rinpol	2154.00		NIST Webbook
tb	852.51	K	Joback Method
tc	1043.79	K	Joback Method
tf	454.33	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1022.14	J/molxK	852.51	Joback Method
cpg	1040.34	J/molxK	884.39	Joback Method
cpg	1057.54	J/molxK	916.27	Joback Method
cpg	1073.80	J/molxK	948.15	Joback Method
cpg	1089.16	J/molxK	980.03	Joback Method
cpg	1103.67	J/molxK	1011.91	Joback Method
cpg	1117.36	J/molxK	1043.79	Joback Method

dvisc	0.0007680	Paxs	454.33	Joback Method
dvisc	0.0002266	Paxs	520.69	Joback Method
dvisc	0.0000881	Paxs	587.06	Joback Method
dvisc	0.0000415	Paxs	653.42	Joback Method
dvisc	0.0000224	Paxs	719.78	Joback Method
dvisc	0.0000135	Paxs	786.15	Joback Method
dvisc	0.0000088	Paxs	852.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C821170&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
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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