Octadecanoic acid, 2-propenyl ester

Other names: Stearic acid, allyl ester
Allyl stearate
Inchi: InChI=1S/C21H40O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21(22)23-20-4-2/h4
InchiKey: HPCIWDZYMSZAEZ-UHFFFAOYSA-N
Formula: C21H40O2
SMILES: C=CCOC(=O)CCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 324.54
CAS: 6289-31-2

Physical Properties

Property code	Value	Unit	Source
gf	-20.14	kJ/mol	Joback Method
hf	-596.14	kJ/mol	Joback Method
hfus	51.65	kJ/mol	Joback Method
hvap	70.83	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	6.977		Crippen Method
mcvol	309.890	ml/mol	McGowan Method
pc	1010.37	kPa	Joback Method
rinpol	2251.00		NIST Webbook
tb	752.85	K	Joback Method
tc	926.96	K	Joback Method
tf	396.83	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.33	J/mol×K	752.85	Joback Method
cpg	962.90	J/mol×K	781.87	Joback Method
cpg	981.53	J/mol×K	810.89	Joback Method
cpg	999.24	J/mol×K	839.91	Joback Method
cpg	1016.06	J/mol×K	868.93	Joback Method
cpg	1032.03	J/mol×K	897.94	Joback Method

cpg	1047.16	J/mol×K	926.96	Joback Method
dvisc	0.0014892	Pa×s	396.83	Joback Method
dvisc	0.0006370	Pa×s	456.17	Joback Method
dvisc	0.0003313	Pa×s	515.50	Joback Method
dvisc	0.0001972	Pa×s	574.84	Joback Method
dvisc	0.0001293	Pa×s	634.18	Joback Method
dvisc	0.0000912	Pa×s	693.51	Joback Method
dvisc	0.0000679	Pa×s	752.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6289312&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
mcvol:	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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