2-Heptenoic acid, undec-2-en-1-yl ester

Inchi: InChI=1S/C18H32O2/c1-3-5-7-9-10-11-12-13-15-17-20-18(19)16-14-8-6-4-2/h13-16H,3-1
InchiKey: JPBQGOOHZHHKFM-WXUKJITCSA-N
Formula: C18H32O2
SMILES: CCCCC=CC(=O)OCC=CCCCCCCCC
Mol. weight [g/mol]: 280.45

Physical Properties

Property code	Value	Unit	Source
gf	27.20	kJ/mol	Joback Method
hf	-425.21	kJ/mol	Joback Method
hfus	45.57	kJ/mol	Joback Method
hvap	64.73	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.583		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	2272.00		NIST Webbook
rinpol	2272.00		NIST Webbook
tb	695.85	K	Joback Method
tc	872.86	K	Joback Method
tf	354.62	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.84	J/mol×K	695.85	Joback Method
cpg	763.70	J/mol×K	725.35	Joback Method
cpg	780.72	J/mol×K	754.85	Joback Method
cpg	796.93	J/mol×K	784.36	Joback Method
cpg	812.37	J/mol×K	813.86	Joback Method
cpg	827.07	J/mol×K	843.36	Joback Method
cpg	841.08	J/mol×K	872.86	Joback Method
dvisc	0.0017692	Pa×s	354.62	Joback Method

dvisc	0.0007146	Pa×s	411.49	Joback Method
dvisc	0.0003597	Pa×s	468.36	Joback Method
dvisc	0.0002101	Pa×s	525.24	Joback Method
dvisc	0.0001363	Pa×s	582.11	Joback Method
dvisc	0.0000955	Pa×s	638.98	Joback Method
dvisc	0.0000709	Pa×s	695.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406945&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