Pentyl 10-undecenoate

Other names: 10-Undecenoic acid, pentyl ester
pentyl undec-10-enoate
Inchi: InChI=1S/C16H30O2/c1-3-5-7-8-9-10-11-12-14-16(17)18-15-13-6-4-2/h3H,1,4-15H2,2H3
InchiKey: UODPTRHAWGAWQL-UHFFFAOYSA-N
Formula: C16H30O2
SMILES: C=CCCCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]: 254.41
CAS: 18451-96-2

Physical Properties

Property code	Value	Unit	Source
gf	-62.24	kJ/mol	Joback Method
hf	-492.94	kJ/mol	Joback Method
hfus	38.70	kJ/mol	Joback Method
hvap	59.70	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	5.027		Crippen Method
mcvol	239.440	ml/mol	McGowan Method
pc	1406.95	kPa	Joback Method
rinpol	1760.00		NIST Webbook
ripol	2053.00		NIST Webbook
tb	638.45	K	Joback Method
tc	807.79	K	Joback Method
tf	340.48	K	Joback Method
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.09	J/mol×K	638.45	Joback Method
cpg	670.50	J/mol×K	666.67	Joback Method
cpg	687.15	J/mol×K	694.90	Joback Method
cpg	703.06	J/mol×K	723.12	Joback Method
cpg	718.25	J/mol×K	751.34	Joback Method

cpg	732.75	J/mol×K	779.57	Joback Method
cpg	746.55	J/mol×K	807.79	Joback Method
dvisc	0.0023340	Pa×s	340.48	Joback Method
dvisc	0.0010565	Pa×s	390.14	Joback Method
dvisc	0.0005720	Pa×s	439.80	Joback Method
dvisc	0.0003507	Pa×s	489.47	Joback Method
dvisc	0.0002353	Pa×s	539.13	Joback Method
dvisc	0.0001689	Pa×s	588.79	Joback Method
dvisc	0.0001276	Pa×s	638.45	Joback Method

Sources

Joback Method:	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=C18451962&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 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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