(Z)-3-hexenyl undecanoate

Inchi: InChI=1S/C17H32O2/c1-3-5-7-9-10-11-12-13-15-17(18)19-16-14-8-6-4-2/h6,8H,3-5,7,9-1
InchiKey: HLDPXZRNQXKWRH-VURMDHGXSA-N
Formula: C17H32O2
SMILES: CCC=CCCOC(=O)CCCCCCCCCC
Mol. weight [g/mol]: 268.43

Physical Properties

Property code	Value	Unit	Source
gf	-61.44	kJ/mol	Joback Method
hf	-521.79	kJ/mol	Joback Method
hfus	42.77	kJ/mol	Joback Method
hvap	62.55	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.417		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
ripol	2125.00		NIST Webbook
ripol	2125.00		NIST Webbook
tb	668.81	K	Joback Method
tc	841.03	K	Joback Method
tf	348.43	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.95	J/mol×K	668.81	Joback Method
cpg	728.86	J/mol×K	697.51	Joback Method
cpg	745.96	J/mol×K	726.22	Joback Method
cpg	762.28	J/mol×K	754.92	Joback Method
cpg	777.84	J/mol×K	783.62	Joback Method
cpg	792.67	J/mol×K	812.33	Joback Method

cpg	806.79	J/mol×K	841.03	Joback Method
dvisc	0.0020673	Pa×s	348.43	Joback Method
dvisc	0.0008745	Pa×s	401.83	Joback Method
dvisc	0.0004527	Pa×s	455.22	Joback Method
dvisc	0.0002691	Pa×s	508.62	Joback Method
dvisc	0.0001766	Pa×s	562.02	Joback Method
dvisc	0.0001246	Pa×s	615.41	Joback Method
dvisc	0.0000930	Pa×s	668.81	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=R239868&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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