

Hexyl undecanoate

Inchi:	InChI=1S/C17H34O2/c1-3-5-7-9-10-11-12-13-15-17(18)19-16-14-8-6-4-2/h3-16H2,1-2H3
InchiKey:	KZNVUDWSXYNJGE-UHFFFAOYSA-N
Formula:	C17H34O2
SMILES:	CCCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]:	270.45

Physical Properties

Property code	Value	Unit	Source
gf	-141.66	kJ/mol	Joback Method
hf	-639.01	kJ/mol	Joback Method
hfus	42.57	kJ/mol	Joback Method
hvap	62.59	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.641		Crippen Method
mvol	257.830	ml/mol	McGowan Method
pc	1271.87	kPa	Joback Method
rinpol	1862.00		NIST Webbook
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tb	664.65	K	Joback Method
tc	832.26	K	Joback Method
tf	353.51	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.28	J/molxK	664.65	Joback Method
cpg	750.62	J/molxK	692.59	Joback Method
cpg	768.17	J/molxK	720.52	Joback Method
cpg	784.95	J/molxK	748.46	Joback Method
cpg	800.97	J/molxK	776.39	Joback Method
cpg	816.25	J/molxK	804.33	Joback Method
cpg	830.80	J/molxK	832.26	Joback Method
dvisc	0.0022120	Paxs	353.51	Joback Method

dvisc	0.0009695	Paxs	405.37	Joback Method
dvisc	0.0005124	Paxs	457.22	Joback Method
dvisc	0.0003083	Paxs	509.08	Joback Method
dvisc	0.0002038	Paxs	560.94	Joback Method
dvisc	0.0001445	Paxs	612.79	Joback Method
dvisc	0.0001081	Paxs	664.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R543325&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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