

Allyl tridecanoate

Inchi:	InChI=1S/C16H30O2/c1-3-5-6-7-8-9-10-11-12-13-14-16(17)18-15-4-2/h4H,2-3,5-15H2,1
InchiKey:	XVYSUWDBWVPTGL-UHFFFAOYSA-N
Formula:	C16H30O2
SMILES:	C=CCOC(=O)CCCCCCCCCCCC
Mol. weight [g/mol]:	254.41

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	1755.00		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/molxK	638.45	Joback Method
cpg	732.75	J/molxK	779.57	Joback Method
cpg	718.25	J/molxK	751.34	Joback Method
cpg	703.06	J/molxK	723.12	Joback Method
cpg	687.15	J/molxK	694.90	Joback Method
cpg	670.50	J/molxK	666.67	Joback Method
cpg	746.55	J/molxK	807.79	Joback Method
dvisc	0.0001276	Paxs	638.45	Joback Method
dvisc	0.0001689	Paxs	588.79	Joback Method

dvisc	0.0002353	Paxs	539.13	Joback Method
dvisc	0.0003507	Paxs	489.47	Joback Method
dvisc	0.0005720	Paxs	439.80	Joback Method
dvisc	0.0010565	Paxs	390.14	Joback Method
dvisc	0.0023340	Paxs	340.48	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=R541181&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
mccvol:	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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<https://www.chemeo.com/cid/50-832-2/Allyl-tridecanoate.pdf>

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