

Allyl pentadecanoate

Inchi:	InChI=1S/C18H34O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-18(19)20-17-4-2/h4H,2-3,5-1
InchiKey:	VDBFRTPHASGVDU-UHFFFAOYSA-N
Formula:	C18H34O2
SMILES:	C=CCOC(=O)CCCCCCCCCCCCC
Mol. weight [g/mol]:	282.46

Physical Properties

Property code	Value	Unit	Source
gf	-45.40	kJ/mol	Joback Method
hf	-534.22	kJ/mol	Joback Method
hfus	43.88	kJ/mol	Joback Method
hvap	64.15	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.807		Crippen Method
mcvol	267.620	ml/mol	McGowan Method
pc	1224.27	kPa	Joback Method
rinpol	1853.00		NIST Webbook
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tb	684.21	K	Joback Method
tc	853.95	K	Joback Method
tf	363.02	K	Joback Method
vc	1.048	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.80	J/molxK	684.21	Joback Method
cpg	784.09	J/molxK	712.50	Joback Method
cpg	801.56	J/molxK	740.79	Joback Method
cpg	818.22	J/molxK	769.08	Joback Method
cpg	834.11	J/molxK	797.37	Joback Method
cpg	849.23	J/molxK	825.66	Joback Method
cpg	863.62	J/molxK	853.95	Joback Method
dvisc	0.0019864	Paxs	363.02	Joback Method

dvisc	0.0008773	Paxs	416.55	Joback Method
dvisc	0.0004667	Paxs	470.08	Joback Method
dvisc	0.0002825	Paxs	523.62	Joback Method
dvisc	0.0001877	Paxs	577.15	Joback Method
dvisc	0.0001337	Paxs	630.68	Joback Method
dvisc	0.0001004	Paxs	684.21	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=R541161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	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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