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)CCCCCCCCCCCCCC
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
rinpol	1853.00		NIST Webbook
tb	684.21	K	Joback Method
tc	853.95	K	Joback Method
tf	363.02	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.80	J/mol×K	684.21	Joback Method
cpg	849.23	J/mol×K	825.66	Joback Method
cpg	834.11	J/mol×K	797.37	Joback Method
cpg	818.22	J/mol×K	769.08	Joback Method
cpg	801.56	J/mol×K	740.79	Joback Method
cpg	784.09	J/mol×K	712.50	Joback Method
cpg	863.62	J/mol×K	853.95	Joback Method
dvisc	0.0001004	Pa×s	684.21	Joback Method

dvisc	0.0001337	Pa×s	630.68	Joback Method
dvisc	0.0001877	Pa×s	577.15	Joback Method
dvisc	0.0002825	Pa×s	523.62	Joback Method
dvisc	0.0004667	Pa×s	470.08	Joback Method
dvisc	0.0008773	Pa×s	416.55	Joback Method
dvisc	0.0019864	Pa×s	363.02	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R541161&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume