E-9-hexadecenyl acetate

Inchi: InChI=1S/C18H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-18(2)19/h8-9H,3-7,1
InchiKey: VAKBQCYSUVICLV-CMDGGOBGSA-N
Formula: C18H34O2
SMILES: CCCCCCC=CCCCCCCCCOC(C)=O
Mol. weight [g/mol]: 282.46

Physical Properties

Property code	Value	Unit	Source
gf	-53.02	kJ/mol	Joback Method
hf	-542.43	kJ/mol	Joback Method
hfus	45.36	kJ/mol	Joback Method
hvap	64.78	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.807		Crippen Method
mcvol	267.620	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	1998.00		NIST Webbook
rinpol	1998.00		NIST Webbook
ripol	2317.00		NIST Webbook
ripol	2317.00		NIST Webbook
tb	691.69	K	Joback Method
tc	864.16	K	Joback Method
tf	359.70	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.00	J/mol×K	691.69	Joback Method
cpg	786.32	J/mol×K	720.43	Joback Method
cpg	803.81	J/mol×K	749.18	Joback Method
cpg	820.48	J/mol×K	777.92	Joback Method
cpg	836.37	J/mol×K	806.67	Joback Method
cpg	851.50	J/mol×K	835.41	Joback Method

cpg	865.91	J/mol×K	864.16	Joback Method
dvisc	0.0018910	Pa×s	359.70	Joback Method
dvisc	0.0007915	Pa×s	415.03	Joback Method
dvisc	0.0004066	Pa×s	470.36	Joback Method
dvisc	0.0002403	Pa×s	525.70	Joback Method
dvisc	0.0001570	Pa×s	581.03	Joback Method
dvisc	0.0001105	Pa×s	636.36	Joback Method
dvisc	0.0000822	Pa×s	691.69	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R69005&Units=SI
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

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