E-8-METHYL-9-TETRADECEN-1-OL ACETATE

Inchi: InChI=1S/C17H32O2/c1-4-5-6-10-13-16(2)14-11-8-7-9-12-15-19-17(3)18/h10,13,16H,4-9
InchiKey: XAIYESIBSJPKNQ-JLHYYAGUSA-N
Formula: C17H32O2
SMILES: CCCC/C=C/C(C)CCCCCCCOC(C)=O
Mol. weight [g/mol]: 268.44

Physical Properties

Property code	Value	Unit	Source
af	0.7366		Cheméo Relay (1.0)
hf	-631.66	kJ/mol	Cheméo Relay (1.0)
hfus	39.25	kJ/mol	Joback Method
hvap	86.25	kJ/mol	Cheméo Relay (1.0)
ie	8.76	eV	Cheméo Relay (1.0)
log10ws	-5.43		Cheméo Relay (1.0)
logp	5.273		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
tb	562.67	K	Cheméo Relay (1.0)
tc	731.95	K	Cheméo Relay (1.0)
tf	253.41	K	Cheméo Relay (1.0)
vc	0.937	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.36	J/mol×K	668.37	Joback Method
cpg	808.37	J/mol×K	842.81	Joback Method
cpg	794.12	J/mol×K	813.73	Joback Method
cpg	779.14	J/mol×K	784.66	Joback Method
cpg	763.40	J/mol×K	755.59	Joback Method
cpg	746.87	J/mol×K	726.52	Joback Method
cpg	729.53	J/mol×K	697.44	Joback Method
dvisc	0.0002718	Pa×s	500.90	Joback Method
dvisc	0.0000863	Pa×s	668.37	Joback Method

dvisc	0.0001180	Pa×s	612.55	Joback Method
dvisc	0.0001717	Pa×s	556.72	Joback Method
dvisc	0.0027098	Pa×s	333.43	Joback Method
dvisc	0.0004826	Pa×s	445.08	Joback Method
dvisc	0.0010105	Pa×s	389.25	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U130814&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume