13-TETRADECEN-1-OL ACETATE

Other names: 13-tetradecenyl acetate
Inchi: InChI=1S/C16H30O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-16(2)17/h3H,1,4-15H2,2H3
InchiKey: DZXBZPMJYIXTTI-UHFFFAOYSA-N
Formula: C16H30O2
SMILES: C=CCCCCCCCCCCCCOC(C)=O
Mol. weight [g/mol]: 254.41

Physical Properties

Property code	Value	Unit	Source
af	0.7843		Cheméo Relay (1.0)
gf	-62.24	kJ/mol	Joback Method
hf	-589.96	kJ/mol	Cheméo Relay (1.0)
hfus	38.70	kJ/mol	Joback Method
hvap	87.78	kJ/mol	Cheméo Relay (1.0)
ie	9.36	eV	Cheméo Relay (1.0)
log10ws	-5.30		Cheméo Relay (1.0)
logp	5.027		Crippen Method
mcvol	239.440	ml/mol	McGowan Method
pc	1406.95	kPa	Joback Method
rinpol	1805.00		NIST Webbook
rinpol	1805.00		NIST Webbook
ripol	2137.00		NIST Webbook
ripol	2137.00		NIST Webbook
tb	577.62	K	Cheméo Relay (1.0)
tc	742.88	K	Cheméo Relay (1.0)
tf	285.44	K	Cheméo Relay (1.0)
vc	0.908	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.09	J/mol×K	638.45	Joback Method
cpg	746.55	J/mol×K	807.79	Joback Method
cpg	732.75	J/mol×K	779.57	Joback Method

cpg	718.25	J/mol×K	751.34	Joback Method
cpg	703.06	J/mol×K	723.12	Joback Method
cpg	687.15	J/mol×K	694.90	Joback Method
cpg	670.50	J/mol×K	666.67	Joback Method
dvisc	0.0003507	Pa×s	489.47	Joback Method
dvisc	0.0001276	Pa×s	638.45	Joback Method
dvisc	0.0001689	Pa×s	588.79	Joback Method
dvisc	0.0002353	Pa×s	539.13	Joback Method
dvisc	0.0023340	Pa×s	340.48	Joback Method
dvisc	0.0005720	Pa×s	439.80	Joback Method
dvisc	0.0010565	Pa×s	390.14	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56221911&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

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

ie: Ionization energy

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