(E)-3-(E)-13-Octadecadien-1-ol acetate

Inchi: InChI=1S/C20H36O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-20(2)21/h6-7,
InchiKey: NWRSOYAGXTXEMK-QRNOYXLNSA-N
Formula: C20H36O2
SMILES: CCCCC=CCCCCCCCCCC=CCOC(C)=O
Mol. weight [g/mol]: 308.50

Physical Properties

Property code	Value	Unit	Source
af	0.8069		Cheméo Relay (1.0)
hf	-661.86	kJ/mol	Cheméo Relay (1.0)
hfus	50.75	kJ/mol	Joback Method
hvap	103.86	kJ/mol	Cheméo Relay (1.0)
ie	8.74	eV	Cheméo Relay (1.0)
log10ws	-6.39		Cheméo Relay (1.0)
logp	6.363		Crippen Method
mcvol	291.500	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	2078.00		NIST Webbook
rinpol	2000.00		NIST Webbook
ripol	2054.00		NIST Webbook
ripol	2056.00		NIST Webbook
tb	594.30	K	Cheméo Relay (1.0)
tc	769.94	K	Cheméo Relay (1.0)
tf	261.33	K	Cheméo Relay (1.0)
vc	1.072	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.13	J/mol×K	741.61	Joback Method
cpg	880.77	J/mol×K	771.29	Joback Method
cpg	898.51	J/mol×K	800.97	Joback Method
cpg	915.41	J/mol×K	830.65	Joback Method
cpg	931.49	J/mol×K	860.34	Joback Method

cpg	946.80	J/mol×K	890.02	Joback Method
cpg	961.38	J/mol×K	919.70	Joback Method
dvisc	0.0014552	Pa×s	377.16	Joback Method
dvisc	0.0005772	Pa×s	437.90	Joback Method
dvisc	0.0002868	Pa×s	498.64	Joback Method
dvisc	0.0001659	Pa×s	559.38	Joback Method
dvisc	0.0001068	Pa×s	620.13	Joback Method
dvisc	0.0000744	Pa×s	680.87	Joback Method
dvisc	0.0000550	Pa×s	741.61	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R571701&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

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
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