

(E)-2-(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
gf	44.04	kJ/mol	Joback Method
hf	-466.49	kJ/mol	Joback Method
hfus	50.75	kJ/mol	Joback Method
hvap	69.19	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.363		Crippen Method
mcvol	291.500	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	2078.00		NIST Webbook
ripol	2056.00		NIST Webbook
tb	741.61	K	Joback Method
tc	919.70	K	Joback Method
tf	377.16	K	Joback Method
vc	1.139	m3/kmol	Joback Method

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:	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=R571701&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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