

(E)-3-(Z)-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:	VVJPJXKHBZNADP-ZSTZHTMOSA-N
Formula:	C20H36O2
SMILES:	CCCC=CCCCCCCCC=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
mvol	291.500	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
ripol	2000.00		NIST Webbook
ripol	2065.00		NIST Webbook
tb	741.61	K	Joback Method
tc	919.70	K	Joback Method
tf	377.16	K	Joback Method
vc	1.139	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.13	J/molxK	741.61	Joback Method
cpg	880.77	J/molxK	771.29	Joback Method
cpg	898.51	J/molxK	800.97	Joback Method
cpg	915.41	J/molxK	830.65	Joback Method
cpg	931.49	J/molxK	860.34	Joback Method
cpg	946.80	J/molxK	890.02	Joback Method
cpg	961.38	J/molxK	919.70	Joback Method
dvisc	0.0014552	Paxs	377.16	Joback Method

dvisc	0.0005772	Paxs	437.90	Joback Method
dvisc	0.0002868	Paxs	498.64	Joback Method
dvisc	0.0001659	Paxs	559.38	Joback Method
dvisc	0.0001068	Paxs	620.13	Joback Method
dvisc	0.0000744	Paxs	680.87	Joback Method
dvisc	0.0000550	Paxs	741.61	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R571781&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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