cis-7,cis-11-Hexadecadien-1-yl acetate

Other names:	7,11-Hexadecadien-1-ol, acetate, (Z,Z)-
	Z,Z-7,11-Hexadecadien-1-yl acetate
	Z,Z-7,11-Hexadecadien-1-ol acetate
	(7Z,11Z)-7,11-Hexadecadienyl acetate
	(7Z,11Z)-Hexadecadien-1-yl acetate
	Gossyplure (Z,Z)-
	(Z,Z)-Gossyplure
	(7Z,11Z)-hexadecadienyl acetate
	(Z,Z)-hexadeca-7,11-dienyl acetate
Inchi:	InChI=1S/C18H32O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-18(2)19/h6-7,10-11H
InchiKey:	BXJHOKLLMOYSRQ-QOXWLJPHSA-N
Formula:	C18H32O2
SMILES:	CCCCC=CCCC=CCCCCCCOC(C)=O
Mol. weight [g/mol]:	280.45
CAS:	52207-99-5

Physical Properties

Property code	Value	Unit	Source
gf	27.20	kJ/mol	Joback Method
hf	-425.21	kJ/mol	Joback Method
hfus	45.57	kJ/mol	Joback Method
hvap	64.73	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.583		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
tb	695.85	K	Joback Method
tc	872.86	K	Joback Method
tf	354.62	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	745.84	J/mol×K	695.85	Joback Method
cpg	827.07	J/mol×K	843.36	Joback Method
cpg	812.37	J/mol×K	813.86	Joback Method
cpg	796.93	J/mol×K	784.36	Joback Method
cpg	780.72	J/mol×K	754.85	Joback Method
cpg	763.70	J/mol×K	725.35	Joback Method
cpg	841.08	J/mol×K	872.86	Joback Method
dvisc	0.0000709	Pa×s	695.85	Joback Method
dvisc	0.0000955	Pa×s	638.98	Joback Method
dvisc	0.0001363	Pa×s	582.11	Joback Method
dvisc	0.0002101	Pa×s	525.24	Joback Method
dvisc	0.0003597	Pa×s	468.36	Joback Method
dvisc	0.0007146	Pa×s	411.49	Joback Method
dvisc	0.0017692	Pa×s	354.62	Joback Method

Sources

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=C52207995&Units=SI

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

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

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume