

(Z,E)-11,13,15-hexadecatrienyl acetate

Inchi:	InChI=1S/C18H30O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-18(2)19/h3-7H,1,8-1
InchiKey:	LSRIOUSPMIDHBL-DEQVHDEQSA-N
Formula:	C18H30O2
SMILES:	C=CC=CC=CCCCCCCCCCCCOC(C)=O
Mol. weight [g/mol]:	278.43

Physical Properties

Property code	Value	Unit	Source
gf	115.04	kJ/mol	Joback Method
hf	-299.78	kJ/mol	Joback Method
hfus	44.29	kJ/mol	Joback Method
hvap	64.06	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.359		Crippen Method
mvol	259.020	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2088.00		NIST Webbook
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tb	692.53	K	Joback Method
tc	871.47	K	Joback Method
tf	352.86	K	Joback Method
vc	1.008	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.71	J/molxK	692.53	Joback Method
cpg	739.08	J/molxK	722.35	Joback Method
cpg	755.60	J/molxK	752.18	Joback Method
cpg	771.33	J/molxK	782.00	Joback Method
cpg	786.30	J/molxK	811.83	Joback Method
cpg	800.55	J/molxK	841.65	Joback Method
cpg	814.12	J/molxK	871.47	Joback Method
dvisc	0.0017304	Paxs	352.86	Joback Method

dvisc	0.0007136	Paxs	409.47	Joback Method
dvisc	0.0003649	Paxs	466.08	Joback Method
dvisc	0.0002158	Paxs	522.69	Joback Method
dvisc	0.0001414	Paxs	579.31	Joback Method
dvisc	0.0000999	Paxs	635.92	Joback Method
dvisc	0.0000747	Paxs	692.53	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=R406365&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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