

(Z)-12-Hexadecenyl acetate

Inchi:	InChI=1S/C18H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-18(2)19/h5-6H,3-4,7
InchiKey:	MGPBZLCNYHCLEI-WAYWQWQ TSA-N
Formula:	C18H34O2
SMILES:	CCCC=CCCCCCCCCCCCOC(C)=O
Mol. weight [g/mol]:	282.46

Physical Properties

Property code	Value	Unit	Source
gf	-53.02	kJ/mol	Joback Method
hf	-542.43	kJ/mol	Joback Method
hfus	45.36	kJ/mol	Joback Method
hvap	64.78	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.807		Crippen Method
mcvol	267.620	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	1934.00		NIST Webbook
rinpol	2011.00		NIST Webbook
rinpol	2011.00		NIST Webbook
rinpol	1934.00		NIST Webbook
ripol	2339.00		NIST Webbook
ripol	2339.00		NIST Webbook
tb	691.69	K	Joback Method
tc	864.16	K	Joback Method
tf	359.70	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.00	J/molxK	691.69	Joback Method
cpg	851.50	J/molxK	835.41	Joback Method
cpg	836.37	J/molxK	806.67	Joback Method
cpg	820.48	J/molxK	777.92	Joback Method

cpg	803.81	J/mol×K	749.18	Joback Method
cpg	786.32	J/mol×K	720.43	Joback Method
cpg	865.91	J/mol×K	864.16	Joback Method
dvisc	0.0000822	Paxs	691.69	Joback Method
dvisc	0.0001105	Paxs	636.36	Joback Method
dvisc	0.0001570	Paxs	581.03	Joback Method
dvisc	0.0002403	Paxs	525.70	Joback Method
dvisc	0.0004066	Paxs	470.36	Joback Method
dvisc	0.0007915	Paxs	415.03	Joback Method
dvisc	0.0018910	Paxs	359.70	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=R86873&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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