

(E)-6-octadecene

Other names:	(E)-6-Octadecene
Inchi:	InChI=1S/C18H36/c1-3-5-7-9-11-13-15-17-18-16-14-12-10-8-6-4-2/h11,13H,3-10,12,14-16H
InchiKey:	HPDAWHPYUNZJMN-ACCUITESSA-N
Formula:	C18H36
SMILES:	CCCCC=CCCCCCCCCCCC
Mol. weight [g/mol]:	252.48
CAS:	7206-22-6

Physical Properties

Property code	Value	Unit	Source
af	0.7208		Cheméo Relay (1.0)
gf	180.90	kJ/mol	Joback Method
hf	-343.86	kJ/mol	Cheméo Relay (1.0)
hfus	42.58	kJ/mol	Joback Method
hvap	87.00	kJ/mol	Cheméo Relay (1.0)
ie	8.94	eV	Cheméo Relay (1.0)
log10ws	-7.67		Cheméo Relay (1.0)
logp	7.044		Crippen Method
mcvol	260.180	ml/mol	McGowan Method
pc	1194.00	kPa	Joback Method
tb	563.30	K	Cheméo Relay (1.0)
tc	733.01	K	Cheméo Relay (1.0)
tf	273.75 ± 2.00	K	NIST Webbook
vc	1.031	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.15	J/mol×K	615.40	Joback Method
cpg	723.88	J/mol×K	642.67	Joback Method
cpg	742.80	J/mol×K	669.95	Joback Method
cpg	760.91	J/mol×K	697.22	Joback Method
cpg	778.26	J/mol×K	724.50	Joback Method
cpg	794.87	J/mol×K	751.77	Joback Method

cpg	810.77	J/mol×K	779.04	Joback Method
dvisc	0.0041393	Pa×s	287.54	Joback Method
dvisc	0.0013772	Pa×s	342.18	Joback Method
dvisc	0.0006204	Pa×s	396.83	Joback Method
dvisc	0.0003390	Pa×s	451.47	Joback Method
dvisc	0.0002111	Pa×s	506.11	Joback Method
dvisc	0.0001441	Pa×s	560.76	Joback Method
dvisc	0.0001053	Pa×s	615.40	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7206226&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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