(E)-2-octadecene

Other names: (E)-2-Octadecene
2-octadecene (E)
Inchi: InChI=1S/C18H36/c1-3-5-7-9-11-13-15-17-18-16-14-12-10-8-6-4-2/h3,5H,4,6-18H2,1-2H
InchiKey: KUQIWULJSBTNPX-HWKANZROSA-N
Formula: C18H36
SMILES: CC=CCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 252.48
CAS: 7206-18-0

Physical Properties

Property code	Value	Unit	Source
af	0.7383		Cheméo Relay (1.0)
gf	180.90	kJ/mol	Joback Method
hf	-337.83	kJ/mol	Cheméo Relay (1.0)
hfus	42.58	kJ/mol	Joback Method
hvap	90.16	kJ/mol	Cheméo Relay (1.0)
ie	9.11	eV	Cheméo Relay (1.0)
log10ws	-7.70		Cheméo Relay (1.0)
logp	7.044		Crippen Method
mcvol	260.180	ml/mol	McGowan Method
pc	1194.00	kPa	Joback Method
tb	568.38	K	Cheméo Relay (1.0)
tc	733.61	K	Cheméo Relay (1.0)
tf	286.40 ± 2.00	K	NIST Webbook
vc	1.027	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=C7206180&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