

1,3-Octadiene (e & z)

Inchi:	InChI=1S/2C8H14/c2*1-3-5-7-8-6-4-2/h2*3,5,7H,1,4,6,8H2,2H3/b7-5+;7-5-
InchiKey:	AHXYUFDHOFVJLM-QUMALBNYSA-N
Formula:	C16H28
SMILES:	C=CC=CCCC.C=CC=CCCC
Mol. weight [g/mol]:	220.39

Physical Properties

Property code	Value	Unit	Source
gf	315.20	kJ/mol	Joback Method
hf	0.11	kJ/mol	Joback Method
hfus	31.68	kJ/mol	Joback Method
hvap	50.08	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	5.838		Crippen Method
mcvol	229.960	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
tb	568.56	K	Joback Method
tc	749.31	K	Joback Method
tf	223.66	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.24	J/molxK	568.56	Joback Method
cpg	572.07	J/molxK	598.69	Joback Method
cpg	591.02	J/molxK	628.81	Joback Method
cpg	609.12	J/molxK	658.94	Joback Method
cpg	626.38	J/molxK	689.06	Joback Method
cpg	642.80	J/molxK	719.19	Joback Method
cpg	658.42	J/molxK	749.31	Joback Method
dvisc	0.0279076	Paxs	223.66	Joback Method
dvisc	0.0027186	Paxs	281.14	Joback Method
dvisc	0.0005839	Paxs	338.63	Joback Method

dvisc	0.0001960	Paxs	396.11	Joback Method
dvisc	0.0000868	Paxs	453.59	Joback Method
dvisc	0.0000461	Paxs	511.08	Joback Method
dvisc	0.0000279	Paxs	568.56	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=B6009789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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