

1,6-Octadiene, (E)-

Other names:	(6E)-1,6-Octadiene 1,trans-6-octadiene
Inchi:	InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h3-4,6H,1,5,7-8H2,2H3/b6-4+
InchiKey:	RJUCIROUEDJQIB-GQCTYLIASA-N
Formula:	C8H14
SMILES:	C=CCCCC=CC
Mol. weight [g/mol]:	110.20
CAS:	19036-81-8

Physical Properties

Property code	Value	Unit	Source
gf	184.54	kJ/mol	Joback Method
hf	34.20	kJ/mol	Joback Method
hfus	15.40	kJ/mol	Joback Method
hvap	32.69	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.919		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	779.00		NIST Webbook
rinpol	779.30		NIST Webbook
rinpol	783.30		NIST Webbook
rinpol	779.80		NIST Webbook
tb	383.28	K	Joback Method
tc	558.73	K	Joback Method
tf	173.08	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.47	J/molxK	383.28	Joback Method
cpg	215.81	J/molxK	412.52	Joback Method
cpg	227.59	J/molxK	441.76	Joback Method

cpg	238.82	J/molxK	471.01	Joback Method
cpg	249.52	J/molxK	500.25	Joback Method
cpg	259.71	J/molxK	529.49	Joback Method
cpg	269.43	J/molxK	558.73	Joback Method
dvisc	0.0043022	Paxs	173.08	Joback Method
dvisc	0.0016670	Paxs	208.11	Joback Method
dvisc	0.0008489	Paxs	243.15	Joback Method
dvisc	0.0005124	Paxs	278.18	Joback Method
dvisc	0.0003462	Paxs	313.21	Joback Method
dvisc	0.0002531	Paxs	348.25	Joback Method
dvisc	0.0001960	Paxs	383.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19036818&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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