

1,cis-3-octadiene

Other names:	1,3-Octadiene, cis
Inchi:	InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h3,5,7H,1,4,6,8H2,2H3/b7-5-
InchiKey:	QTYUSOHYEPOHLV-ALCCZGGFSA-N
Formula:	C8H14
SMILES:	C=CC=CCCCC
Mol. weight [g/mol]:	110.20

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	810.90		NIST Webbook
rinpol	810.50		NIST Webbook
rinpol	810.50		NIST Webbook
rinpol	816.00		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/mol×K	383.28	Joback Method
cpg	215.81	J/mol×K	412.52	Joback Method
cpg	227.59	J/mol×K	441.76	Joback Method
cpg	238.82	J/mol×K	471.01	Joback Method
cpg	249.52	J/mol×K	500.25	Joback Method

cpg	259.71	J/mol×K	529.49	Joback Method
cpg	269.43	J/mol×K	558.73	Joback Method
dvisc	0.0043022	Pa×s	173.08	Joback Method
dvisc	0.0016670	Pa×s	208.11	Joback Method
dvisc	0.0008489	Pa×s	243.15	Joback Method
dvisc	0.0005124	Pa×s	278.18	Joback Method
dvisc	0.0003462	Pa×s	313.21	Joback Method
dvisc	0.0002531	Pa×s	348.25	Joback Method
dvisc	0.0001960	Pa×s	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=R147269&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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