

trans-2,cis-5-octadiene

Other names:	2,5-Octadiene, (E,Z)
Inchi:	InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h3,5-6,8H,4,7H2,1-2H3/b5-3+,8-6-
InchiKey:	GDDAJHJRAKOILH-GMWFMGJWSA-N
Formula:	C8H14
SMILES:	CC=CCC=CCC
Mol. weight [g/mol]:	110.20

Physical Properties

Property code	Value	Unit	Source
gf	176.92	kJ/mol	Joback Method
hf	25.99	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	33.32	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.919		Crippen Method
mcpvol	114.980	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
rinpol	792.70		NIST Webbook
rinpol	796.90		NIST Webbook
rinpol	793.40		NIST Webbook
tb	390.76	K	Joback Method
tc	571.58	K	Joback Method
tf	169.76	K	Joback Method
vc	0.444	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.62	J/mol×K	390.76	Joback Method
cpg	216.35	J/mol×K	420.90	Joback Method
cpg	228.43	J/mol×K	451.03	Joback Method
cpg	239.90	J/mol×K	481.17	Joback Method
cpg	250.79	J/mol×K	511.30	Joback Method
cpg	261.13	J/mol×K	541.44	Joback Method

cpg	270.94	J/mol×K	571.58	Joback Method
dvisc	0.0049045	Paxs	169.76	Joback Method
dvisc	0.0016869	Paxs	206.59	Joback Method
dvisc	0.0008014	Paxs	243.43	Joback Method
dvisc	0.0004630	Paxs	280.26	Joback Method
dvisc	0.0003039	Paxs	317.09	Joback Method
dvisc	0.0002177	Paxs	353.93	Joback Method
dvisc	0.0001661	Paxs	390.76	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R147501&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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