

trans-2,cis-5-nonadiene

Inchi:	InChI=1S/C9H16/c1-3-5-7-9-8-6-4-2/h3,5,8-9H,4,6-7H2,1-2H3/b5-3+,9-8-
InchiKey:	NMFOAHIHPAPYJJ-QRSZSCANSA-N
Formula:	C9H16
SMILES:	CC=CCC=CCCC
Mol. weight [g/mol]:	124.22

Physical Properties

Property code	Value	Unit	Source
gf	185.34	kJ/mol	Joback Method
hf	5.35	kJ/mol	Joback Method
hfus	19.47	kJ/mol	Joback Method
hvap	35.54	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.309		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	887.90		NIST Webbook
tb	413.64	K	Joback Method
tc	593.38	K	Joback Method
tf	181.03	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.26	J/mol×K	413.64	Joback Method
cpg	257.07	J/mol×K	443.60	Joback Method
cpg	270.20	J/mol×K	473.55	Joback Method
cpg	282.68	J/mol×K	503.51	Joback Method
cpg	294.54	J/mol×K	533.47	Joback Method
cpg	305.81	J/mol×K	563.42	Joback Method
cpg	316.52	J/mol×K	593.38	Joback Method
dvisc	0.0052511	Pa×s	181.03	Joback Method
dvisc	0.0017800	Pa×s	219.80	Joback Method

dvisc	0.0008346	Pa×s	258.57	Joback Method
dvisc	0.0004768	Pa×s	297.33	Joback Method
dvisc	0.0003099	Pa×s	336.10	Joback Method
dvisc	0.0002202	Pa×s	374.87	Joback Method
dvisc	0.0001668	Pa×s	413.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R250023&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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