

trans-2,cis-7-nonadiene

Inchi:	InChI=1S/C9H16/c1-3-5-7-9-8-6-4-2/h3-6H,7-9H2,1-2H3/b5-3-,6-4+
InchiKey:	MAMCJGWPGQJKLS-CIIODKQPSA-N
Formula:	C9H16
SMILES:	CC=CCCC=CC
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	897.00		NIST Webbook
rinpol	897.00		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/molxK	413.64	Joback Method
cpg	305.81	J/molxK	563.42	Joback Method
cpg	294.54	J/molxK	533.47	Joback Method
cpg	282.68	J/molxK	503.51	Joback Method
cpg	270.20	J/molxK	473.55	Joback Method
cpg	257.07	J/molxK	443.60	Joback Method
cpg	316.52	J/molxK	593.38	Joback Method
dvisc	0.0001668	Paxs	413.64	Joback Method

dvisc	0.0002202	Paxs	374.87	Joback Method
dvisc	0.0003099	Paxs	336.10	Joback Method
dvisc	0.0004768	Paxs	297.33	Joback Method
dvisc	0.0008346	Paxs	258.57	Joback Method
dvisc	0.0017800	Paxs	219.80	Joback Method
dvisc	0.0052511	Paxs	181.03	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=R250063&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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