

2,4-Heptadiene, (Z,E)

Other names:	cis-2,trans-4-heptadiene
Inchi:	InChI=1S/C7H12/c1-3-5-7-6-4-2/h3,5-7H,4H2,1-2H3/b5-3-,7-6+
InchiKey:	XTJLXXCARCJVPJ-AIJKMKQJSA-N
Formula:	C7H12
SMILES:	CC=CC=CCC
Mol. weight [g/mol]:	96.17

Physical Properties

Property code	Value	Unit	Source
gf	168.50	kJ/mol	Joback Method
hf	46.63	kJ/mol	Joback Method
hfus	14.29	kJ/mol	Joback Method
hvap	31.09	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.529		Crippen Method
mcpvol	100.890	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	751.10		NIST Webbook
rinpol	746.50		NIST Webbook
rinpol	751.10		NIST Webbook
tb	367.88	K	Joback Method
tc	549.48	K	Joback Method
tf	158.49	K	Joback Method
vc	0.388	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.24	J/mol×K	367.88	Joback Method
cpg	218.14	J/mol×K	519.21	Joback Method
cpg	208.84	J/mol×K	488.95	Joback Method
cpg	199.03	J/mol×K	458.68	Joback Method
cpg	188.68	J/mol×K	428.41	Joback Method
cpg	177.76	J/mol×K	398.15	Joback Method

cpg	226.95	J/mol×K	549.48	Joback Method
dvisc	0.0001609	Paxs	367.88	Joback Method
dvisc	0.0002093	Paxs	332.98	Joback Method
dvisc	0.0002894	Paxs	298.08	Joback Method
dvisc	0.0004362	Paxs	263.19	Joback Method
dvisc	0.0007452	Paxs	228.29	Joback Method
dvisc	0.0015445	Paxs	193.39	Joback Method
dvisc	0.0044130	Paxs	158.49	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=R147432&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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