

1,trans-4-Heptadiene

Other names:	1,4-Heptadiene, E 1,4-Heptadiene, trans
Inchi:	InChI=1S/C7H12/c1-3-5-7-6-4-2/h3,6-7H,1,4-5H2,2H3/b7-6+
InchiKey:	FMAMSYJPXSEYSW-VOTSOKGWSA-N
Formula:	C7H12
SMILES:	C=CCC=CCC
Mol. weight [g/mol]:	96.17

Physical Properties

Property code	Value	Unit	Source
gf	176.12	kJ/mol	Joback Method
hf	54.84	kJ/mol	Joback Method
hfus	12.81	kJ/mol	Joback Method
hvap	30.46	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.529		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	677.20		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	674.00		NIST Webbook
tb	360.40	K	Joback Method
tc	536.35	K	Joback Method
tf	161.81	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.57	J/molxK	360.40	Joback Method
cpg	217.10	J/molxK	507.02	Joback Method
cpg	207.96	J/molxK	477.70	Joback Method
cpg	198.35	J/molxK	448.37	Joback Method
cpg	188.27	J/molxK	419.05	Joback Method

cpg	177.68	J/mol×K	389.72	Joback Method
cpg	225.80	J/mol×K	536.35	Joback Method
dvisc	0.0001889	Paxs	360.40	Joback Method
dvisc	0.0002418	Paxs	327.30	Joback Method
dvisc	0.0003273	Paxs	294.20	Joback Method
dvisc	0.0004784	Paxs	261.11	Joback Method
dvisc	0.0007806	Paxs	228.01	Joback Method
dvisc	0.0015040	Paxs	194.91	Joback Method
dvisc	0.0037899	Paxs	161.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R147343&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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