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:	FMAMSYPJXSEYSW-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	674.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	677.20		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/mol×K	360.40	Joback Method
cpg	177.68	J/mol×K	389.72	Joback Method
cpg	188.27	J/mol×K	419.05	Joback Method
cpg	198.35	J/mol×K	448.37	Joback Method
cpg	207.96	J/mol×K	477.70	Joback Method

cpg	217.10	J/mol×K	507.02	Joback Method
cpg	225.80	J/mol×K	536.35	Joback Method
dvisc	0.0037899	Pa×s	161.81	Joback Method
dvisc	0.0015040	Pa×s	194.91	Joback Method
dvisc	0.0007806	Pa×s	228.01	Joback Method
dvisc	0.0004784	Pa×s	261.11	Joback Method
dvisc	0.0003273	Pa×s	294.20	Joback Method
dvisc	0.0002418	Pa×s	327.30	Joback Method
dvisc	0.0001889	Pa×s	360.40	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/ci990307l
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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