2,5-Heptadiene, (E,E)-

Other names:	trans,trans-2,5-Heptadiene
	(2E,5E)-2,5-Heptadiene
	trans-2,trans-5-Heptadiene
	2,5-Heptadiene, (2E,5E)-
Inchi:	InChI=1S/C7H12/c1-3-5-7-6-4-2/h3-6H,7H2,1-2H3/b5-3+,6-4+
InchiKey:	JAGYXYUAYDLKNO-GGWOSOGESA-N
Formula:	C7H12
SMILES:	CC=CCC=CC
Mol. weight [g/mol]:	96.17
CAS:	39619-60-8

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
mcvol	100.890	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	708.30		NIST Webbook
rinpol	705.10		NIST Webbook
rinpol	716.40		NIST Webbook
rinpol	708.30		NIST Webbook
tb	367.88	K	Joback Method
tc	549.48	K	Joback Method
tf	158.49	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.24	J/mol×K	367.88	Joback Method

cpg	177.76	J/mol×K	398.15	Joback Method
cpg	188.68	J/mol×K	428.41	Joback Method
cpg	199.03	J/mol×K	458.68	Joback Method
cpg	208.84	J/mol×K	488.95	Joback Method
cpg	218.14	J/mol×K	519.21	Joback Method
cpg	226.95	J/mol×K	549.48	Joback Method
dvisc	0.0044130	Pa×s	158.49	Joback Method
dvisc	0.0015445	Pa×s	193.39	Joback Method
dvisc	0.0007452	Pa×s	228.29	Joback Method
dvisc	0.0004362	Pa×s	263.19	Joback Method
dvisc	0.0002894	Pa×s	298.08	Joback Method
dvisc	0.0002093	Pa×s	332.98	Joback Method
dvisc	0.0001609	Pa×s	367.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39619608&Units=SI

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