1,3,6-Octatriene, E,Z

Other names: (E,Z)-1,3,6-octatriene
Inchi: InChI=1S/C8H12/c1-3-5-7-8-6-4-2/h3-7H,1,8H2,2H3/b6-4-,7-5+
InchiKey: PKHBEGZTQNOZLP-XGXWUAJZSA-N
Formula: C8H12
SMILES: C=CC=CCC=CC
Mol. weight [g/mol]: 108.18

Physical Properties

Property code	Value	Unit	Source
gf	264.76	kJ/mol	Joback Method
hf	151.42	kJ/mol	Joback Method
hfus	15.60	kJ/mol	Joback Method
hvap	32.65	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.695		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	816.00		NIST Webbook
rinpol	816.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1100.00		NIST Webbook
tb	387.44	K	Joback Method
tc	572.16	K	Joback Method
tf	168.00	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.00	J/mol×K	387.44	Joback Method
cpg	201.15	J/mol×K	418.23	Joback Method
cpg	212.62	J/mol×K	449.01	Joback Method
cpg	223.45	J/mol×K	479.80	Joback Method
cpg	233.67	J/mol×K	510.59	Joback Method

cpg	243.32	J/mol×K	541.37	Joback Method
cpg	252.44	J/mol×K	572.16	Joback Method
dvisc	0.0039890	Pa×s	168.00	Joback Method
dvisc	0.0014499	Pa×s	204.57	Joback Method
dvisc	0.0007163	Pa×s	241.15	Joback Method
dvisc	0.0004262	Pa×s	277.72	Joback Method
dvisc	0.0002861	Pa×s	314.29	Joback Method
dvisc	0.0002087	Pa×s	350.87	Joback Method
dvisc	0.0001616	Pa×s	387.44	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R294058&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from: