

1,3,5-Octatriene

Inchi:	InChI=1S/C8H12/c1-3-5-7-8-6-4-2/h3,5-8H,1,4H2,2H3/b7-5+,8-6+
InchiKey:	HOXGZVUCAYFWGR-KQQUZDAGSA-N
Formula:	C8H12
SMILES:	C=CC=CC=CCC
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	879.00		NIST Webbook
rinpol	879.00		NIST Webbook
rinpol	882.00		NIST Webbook
ripol	1094.00		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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.00	J/mol×K	387.44	Joback Method
cpg	243.32	J/mol×K	541.37	Joback Method
cpg	233.67	J/mol×K	510.59	Joback Method
cpg	223.45	J/mol×K	479.80	Joback Method
cpg	212.62	J/mol×K	449.01	Joback Method

cpg	201.15	J/molxK	418.23	Joback Method
cpg	252.44	J/molxK	572.16	Joback Method
dvisc	0.0001616	Paxs	387.44	Joback Method
dvisc	0.0002087	Paxs	350.87	Joback Method
dvisc	0.0002861	Paxs	314.29	Joback Method
dvisc	0.0004262	Paxs	277.72	Joback Method
dvisc	0.0007163	Paxs	241.15	Joback Method
dvisc	0.0014499	Paxs	204.57	Joback Method
dvisc	0.0039890	Paxs	168.00	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R301116&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
mccvol:	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

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