

2,4,6-octatriene

Inchi:	InChI=1S/C8H12/c1-3-5-7-8-6-4-2/h3-8H,1-2H3
InchiKey:	CGMDPTNRMYZTM-UHFFFAOYSA-N
Formula:	C8H12
SMILES:	CC=CC=CC=CC
Mol. weight [g/mol]:	108.18
CAS:	764-75-0

Physical Properties

Property code	Value	Unit	Source
gf	257.14	kJ/mol	Joback Method
hf	143.21	kJ/mol	Joback Method
hfus	17.08	kJ/mol	Joback Method
hvap	33.28	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.695		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
tb	401.00 ± 7.00	K	NIST Webbook
tc	585.28	K	Joback Method
tf	325.70 ± 2.00	K	NIST Webbook
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.98	J/mol×K	394.92	Joback Method
cpg	201.48	J/mol×K	426.65	Joback Method
cpg	213.22	J/mol×K	458.37	Joback Method
cpg	224.26	J/mol×K	490.10	Joback Method
cpg	234.63	J/mol×K	521.83	Joback Method
cpg	244.38	J/mol×K	553.55	Joback Method
cpg	253.55	J/mol×K	585.28	Joback Method
dvisc	0.0046000	Pa×s	164.68	Joback Method
dvisc	0.0014728	Pa×s	203.05	Joback Method

dvisc	0.0006773	Pa×s	241.43	Joback Method
dvisc	0.0003854	Pa×s	279.80	Joback Method
dvisc	0.0002513	Pa×s	318.17	Joback Method
dvisc	0.0001796	Pa×s	356.55	Joback Method
dvisc	0.0001371	Pa×s	394.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C764750&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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