1,3,7-Octatrien-5-yne

Other names:	1,5,7-Octatriene-3-yene
Inchi:	InChI=1S/C8H8/c1-3-5-7-8-6-4-2/h3-5,7H,1-2H2/b7-5+
InchiKey:	DYQVQSUVEDCHDD-FNORWQNLSA-N
Formula:	C8H8
SMILES:	C=CC#CC=CC=C
Mol. weight [g/mol]:	104.15
CAS:	16607-77-5

Physical Properties

Property code	Value	Unit	Source
gf	475.18	kJ/mol	Joback Method
hf	431.93	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	34.17	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	1.918		Crippen Method
mcvol	102.080	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpol	828.00		NIST Webbook
rinpol	822.00		NIST Webbook
tb	388.96	K	Joback Method
tc	595.33	K	Joback Method
tf	277.42	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.60	J/mol×K	560.94	Joback Method
cpg	164.69	J/mol×K	388.96	Joback Method
cpg	175.05	J/mol×K	423.36	Joback Method
cpg	184.79	J/mol×K	457.75	Joback Method
cpg	193.93	J/mol×K	492.15	Joback Method
cpg	202.52	J/mol×K	526.54	Joback Method

cpg	218.19	J/mol×K	595.33	Joback Method
hvapt	35.10	kJ/mol	371.00	NIST Webbook

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=C16607775&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
hvapt:	Enthalpy of vaporization at a given temperature
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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