

3,4-Octadiene

Inchi:	InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h5,8H,3-4,6H2,1-2H3
InchiKey:	YOXGDVVRKJDLCI-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	CCC=C=CCCC
Mol. weight [g/mol]:	110.20
CAS:	34511-01-8

Physical Properties

Property code	Value	Unit	Source
gf	224.98	kJ/mol	Joback Method
hf	71.55	kJ/mol	Joback Method
hfus	18.81	kJ/mol	Joback Method
hvap	33.80	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.908		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
tb	389.87	K	Joback Method
tc	572.92	K	Joback Method
tf	181.35	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.04	J/mol×K	389.87	Joback Method
cpg	221.00	J/mol×K	420.38	Joback Method
cpg	232.49	J/mol×K	450.89	Joback Method
cpg	243.52	J/mol×K	481.39	Joback Method
cpg	254.10	J/mol×K	511.90	Joback Method
cpg	264.25	J/mol×K	542.41	Joback Method
cpg	273.98	J/mol×K	572.92	Joback Method

Sources

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=C34511018&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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