

C2H5CH=CHCH=CH2

Other names:	1,3-Hexadiene,c&t 1,3-Hexadiene 1,3-Hexadiene cis + trans 1,3-Hexadiene(c,t) cis,trans-hexa-1,3-diene
Inchi:	InChI=1S/C6H10/c1-3-5-6-4-2/h3,5-6H,1,4H2,2H3
InchiKey:	AHAREKHAZNPPMI-UHFFFAOYSA-N
Formula:	C6H10
SMILES:	C=CC=CCC
Mol. weight [g/mol]:	82.14
CAS:	592-48-3

Physical Properties

Property code	Value	Unit	Source
gf	167.70	kJ/mol	Joback Method
hf	75.48	kJ/mol	Joback Method
hfus	10.22	kJ/mol	Joback Method
hvap	28.24	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.139		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
rinpol	618.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	619.00		NIST Webbook
rinpol	598.00		NIST Webbook
tb	337.52	K	Joback Method
tc	513.57	K	Joback Method
tf	150.54	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.12	J/mol×K	337.52	Joback Method
cpg	141.86	J/mol×K	366.86	Joback Method
cpg	151.13	J/mol×K	396.20	Joback Method
cpg	159.96	J/mol×K	425.54	Joback Method
cpg	168.36	J/mol×K	454.89	Joback Method
cpg	176.34	J/mol×K	484.23	Joback Method
cpg	183.93	J/mol×K	513.57	Joback Method
dvisc	0.0031761	Pa×s	150.54	Joback Method
dvisc	0.0012964	Pa×s	181.70	Joback Method
dvisc	0.0006879	Pa×s	212.87	Joback Method
dvisc	0.0004292	Pa×s	244.03	Joback Method
dvisc	0.0002980	Pa×s	275.19	Joback Method
dvisc	0.0002228	Pa×s	306.36	Joback Method
dvisc	0.0001758	Pa×s	337.52	Joback Method
hvapt	32.10	kJ/mol	309.00	NIST Webbook

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=C592483&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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