

1,5-Hexadiene, 2-methyl-

Other names:	2-METHYLDIALLYL 2-Methyl-1,5-hexadiene 2-methylhexa-1,5-diene 5-METHYLDIALLYL <chem>CH2=C(CH3)CH2CH2CH=CH2</chem>
Inchi:	InChI=1S/C7H12/c1-4-5-6-7(2)3/h4H,1-2,5-6H2,3H3
InchiKey:	SLQMKNPIYMOEGB-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	<chem>C=CCCC(=C)C</chem>
Mol. weight [g/mol]:	96.17
CAS:	4049-81-4

Physical Properties

Property code	Value	Unit	Source
gf	175.19	kJ/mol	Joback Method
hf	53.26	kJ/mol	Joback Method
hfus	10.02	kJ/mol	Joback Method
hvap	29.92	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.529		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	666.70		NIST Webbook
rinpol	668.70		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	662.10		NIST Webbook
rinpol	663.00		NIST Webbook
rinpol	669.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	662.10		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	669.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	668.70		NIST Webbook

rinpol	663.00		NIST Webbook
tb	360.00 ± 4.00	K	NIST Webbook
tb	361.25 ± 0.50	K	NIST Webbook
tb	362.00 ± 0.15	K	NIST Webbook
tc	526.72	K	Joback Method
tf	144.27 ± 0.30	K	NIST Webbook
vc	0.391	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.02	J/mol×K	352.80	Joback Method
cpg	177.89	J/mol×K	381.79	Joback Method
cpg	188.29	J/mol×K	410.77	Joback Method
cpg	198.24	J/mol×K	439.76	Joback Method
cpg	207.75	J/mol×K	468.74	Joback Method
cpg	216.83	J/mol×K	497.73	Joback Method
cpg	225.51	J/mol×K	526.72	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56955e+01
Coeff. B	-3.52720e+03
Coeff. C	-4.15770e+01
Temperature range (K), min.	270.50
Temperature range (K), max.	381.26

Sources

KDB:	https://www.thermo.com/files/research/kdb/mol/mol388.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4049814&Units=SI

The Yaws Handbook of Vapor

Pressure:
Crippen Method:

Crippen Method:

Joback Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

https://en.wikipedia.org/wiki/Joback_method

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
pvap:	Vapor 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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