2-Methyl-1,5-hexadiene

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

Physical Properties

Property code	Value	Unit	Source
af	0.2541		Cheméo Relay (1.0)
gf	175.19	kJ/mol	Joback Method
hf	27.05	kJ/mol	Cheméo Relay (1.0)
hfus	10.02	kJ/mol	Joback Method
hvap	34.89	kJ/mol	Cheméo Relay (1.0)
ie	9.22	eV	Cheméo Relay (1.0)
log10ws	-3.17		Cheméo Relay (1.0)
logp	2.529		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	665.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	663.00		NIST Webbook
rinpol	669.00		NIST Webbook
rinpol	668.70		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	669.00		NIST Webbook
rinpol	666.70		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	662.10		NIST Webbook
rinpol	668.70		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	662.10		NIST Webbook
rinpol	661.00		NIST Webbook

tb	361.25 ± 0.50	K	NIST Webbook
tb	362.00 ± 0.15	K	NIST Webbook
tb	360.00 ± 4.00	K	NIST Webbook
tc	527.34	K	Cheméo Relay (1.0)
tf	144.27 ± 0.30	K	NIST Webbook
vc	0.368	m3/kmol	Cheméo Relay (1.0)

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(Pvp) = 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

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol388.mol

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4049814&Units=SI

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

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Cheméo Relay (1.0, beta):	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0):	
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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