

1,2-Heptadiene

Other names:	Butylallene
Inchi:	InChI=1S/C7H12/c1-3-5-7-6-4-2/h5H,1,4,6-7H2,2H3
InchiKey:	OEMWTWLQGRYBGM-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	C=C=CCCCC
Mol. weight [g/mol]:	96.17
CAS:	2384-90-9

Physical Properties

Property code	Value	Unit	Source
gf	224.18	kJ/mol	Joback Method
hf	100.40	kJ/mol	Joback Method
hfus	14.74	kJ/mol	Joback Method
hvap	30.94	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.518		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	376.90 ± 4.00	K	NIST Webbook
tc	537.66	K	Joback Method
tf	173.40	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.18	J/mol×K	359.51	Joback Method
cpg	183.32	J/mol×K	389.20	Joback Method
cpg	193.12	J/mol×K	418.89	Joback Method
cpg	202.59	J/mol×K	448.58	Joback Method
cpg	211.73	J/mol×K	478.28	Joback Method
cpg	220.54	J/mol×K	507.97	Joback Method
cpg	229.02	J/mol×K	537.66	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57638e+01
Coeff. B	-3.68343e+03
Coeff. C	-4.64150e+01
Temperature range (K), min.	284.42
Temperature range (K), max.	398.82

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=C2384909&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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