1,6-Heptadiene

Other names: CH2=CH(CH2)3CH=CH2
Inchi: InChI=1S/C7H12/c1-3-5-7-6-4-2/h3-4H,1-2,5-7H2
InchiKey: GEAWFZNTIFJMHR-UHFFFAOYSA-N
Formula: C7H12
SMILES: C=CCCCC=C
Mol. weight [g/mol]: 96.17
CAS: 3070-53-9

Physical Properties

Property code	Value	Unit	Source
gf	183.74	kJ/mol	Joback Method
hf	63.05	kJ/mol	Joback Method
hfus	11.33	kJ/mol	Joback Method
hvap	29.84	kJ/mol	Joback Method
ie	9.52 ± 0.02	eV	NIST Webbook
log10ws	-2.46		Crippen Method
logp	2.529		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinpol	665.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	677.40		NIST Webbook
rinpol	676.00		NIST Webbook
rinpol	668.30		NIST Webbook
rinpol	664.80		NIST Webbook
rinpol	663.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	674.00		NIST Webbook
tb	362.70	K	NIST Webbook
tb	363.16 ± 1.00	K	NIST Webbook
tb	362.20 ± 1.00	K	NIST Webbook
tc	523.33	K	Joback Method
tf	143.80 ± 2.00	K	NIST Webbook

vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.99	J/mol×K	352.92	Joback Method
cpg	177.68	J/mol×K	381.32	Joback Method
cpg	187.91	J/mol×K	409.72	Joback Method
cpg	197.71	J/mol×K	438.12	Joback Method
cpg	207.08	J/mol×K	466.53	Joback Method
cpg	216.05	J/mol×K	494.93	Joback Method
cpg	224.62	J/mol×K	523.33	Joback Method
dvisc	0.0033042	Pa×s	165.13	Joback Method
dvisc	0.0014702	Pa×s	196.43	Joback Method
dvisc	0.0008173	Pa×s	227.73	Joback Method
dvisc	0.0005236	Pa×s	259.02	Joback Method
dvisc	0.0003692	Pa×s	290.32	Joback Method
dvisc	0.0002787	Pa×s	321.62	Joback Method
dvisc	0.0002211	Pa×s	352.92	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52909e+01
Coeff. B	-3.42306e+03
Coeff. C	-4.19670e+01
Temperature range (K), min.	270.12
Temperature range (K), max.	384.98

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=C3070539&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
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
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