2,4-Heptadiene

Inchi: InChI=1S/C7H12/c1-3-5-7-6-4-2/h3,5-7H,4H2,1-2H3
InchiKey: XTJLXXCARCJVPJ-UHFFFAOYSA-N
Formula: C7H12
SMILES: CC=CC=CCC
Mol. weight [g/mol]: 96.17
CAS: 628-72-8

Physical Properties

Property code	Value	Unit	Source
gf	168.50	kJ/mol	Joback Method
hf	46.63	kJ/mol	Joback Method
hfus	14.29	kJ/mol	Joback Method
hvap	31.09	kJ/mol	Joback Method
ie	8.17	eV	NIST Webbook
log10ws	-2.46		Crippen Method
logp	2.529		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	750.00		NIST Webbook
tb	377.00 ± 2.00	K	NIST Webbook
tb	378.00 ± 3.00	K	NIST Webbook
tb	382.80 ± 2.00	K	NIST Webbook
tb	382.60 ± 2.00	K	NIST Webbook
tb	381.20	K	NIST Webbook
tc	549.48	K	Joback Method
tf	158.49	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.24	J/mol×K	367.88	Joback Method
cpg	218.14	J/mol×K	519.21	Joback Method
cpg	208.84	J/mol×K	488.95	Joback Method

cpg	199.03	J/mol×K	458.68	Joback Method
cpg	188.68	J/mol×K	428.41	Joback Method
cpg	177.76	J/mol×K	398.15	Joback Method
cpg	226.95	J/mol×K	549.48	Joback Method
dvisc	0.0001609	Pa×s	367.88	Joback Method
dvisc	0.0002093	Pa×s	332.98	Joback Method
dvisc	0.0002894	Pa×s	298.08	Joback Method
dvisc	0.0004362	Pa×s	263.19	Joback Method
dvisc	0.0007452	Pa×s	228.29	Joback Method
dvisc	0.0015445	Pa×s	193.39	Joback Method
dvisc	0.0044130	Pa×s	158.49	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55530e+01
Coeff. B	-3.65317e+03
Coeff. C	-4.71100e+01
Temperature range (K), min.	286.42
Temperature range (K), max.	403.81

Sources

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
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=C628728&Units=SI

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