Heptane, 4-methylene-

Other names:	1-Pentene, 2-propyl-
	2-Propyl-1-pentene
	2-Propylpent-1-ene
Inchi:	InChI=1S/C8H16/c1-4-6-8(3)7-5-2/h3-7H2,1-2H3
InchiKey:	FYUUBXZYRPRIHC-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	C=C(CCC)CCC
Mol. weight [g/mol]:	112.21
CAS:	15918-08-8

Physical Properties

Property code	Value	Unit	Source
gf	95.77	kJ/mol	Joback Method
hf	-92.81	kJ/mol	Joback Method
hfus	13.89	kJ/mol	Joback Method
hvap	39.30	kJ/mol	NIST Webbook
log10ws	-3.02		Crippen Method
logp	3.143		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinpol	778.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	778.00		NIST Webbook
tb	379.00	K	Joback Method
tc	549.05	K	Joback Method
tf	164.20	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.72	J/mol×K	379.00	Joback Method
cpg	230.42	J/mol×K	407.34	Joback Method
cpg	242.63	J/mol×K	435.68	Joback Method
cpg	254.35	J/mol×K	464.02	Joback Method
cpg	265.60	J/mol×K	492.37	Joback Method
cpg	276.40	J/mol×K	520.71	Joback Method
cpg	286.75	J/mol×K	549.05	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40452e+01
Coeff. B	-3.25219e+03
Coeff. C	-4.83620e+01
Temperature range (K), min.	284.75
Temperature range (K), max.	420.73

Sources

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

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol320.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15918088&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume