1-Heptene, 2-methyl-

Other names: 2-Methyl-1-heptene
2-Methylhept-1-ene
Inchi: InChI=1S/C8H16/c1-4-5-6-7-8(2)3/h2,4-7H2,1,3H3
InchiKey: RCBGGJURENJHKV-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=C(C)CCCCC
Mol. weight [g/mol]: 112.21
CAS: 15870-10-7

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	784.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	787.50		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	784.30		NIST Webbook
rinpol	774.90		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	776.40		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	782.00		NIST Webbook

rinpol	776.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	787.50		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	782.00		NIST Webbook
tb	392.50 ± 1.00	K	NIST Webbook
tb	393.15 ± 2.00	K	NIST Webbook
tb	392.65 ± 0.50	K	NIST Webbook
tb	393.15 ± 2.00	K	NIST Webbook
tb	392.45 ± 0.50	K	NIST Webbook
tb	392.75 ± 0.40	K	NIST Webbook
tb	391.65 ± 1.00	K	NIST Webbook
tb	389.65 ± 3.00	K	NIST Webbook
tb	392.00 ± 3.00	K	NIST Webbook
tb	392.50	K	NIST Webbook
tb	392.37 ± 0.30	K	NIST Webbook
tb	392.45 ± 0.50	K	NIST Webbook
tb	391.65 ± 1.00	K	NIST Webbook
tc	567.50	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	183.01 ± 0.30	K	NIST Webbook
tf	183.05 ± 0.50	K	NIST Webbook
tf	183.01 ± 0.30	K	NIST Webbook
tf	183.01 ± 1.00	K	NIST Webbook
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	1.41848e+01
Coeff. B	-3.23383e+03
Coeff. C	-5.39600e+01
Temperature range (K), min.	286.66
Temperature range (K), max.	418.41

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

Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons: https://www.doi.org/10.1021/je0341357

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol256.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15870107&Units=SI

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