2-METHYL-1-HEPTENE

Other names: 1-heptene, 2-methyl-
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]: 112.22
CAS: 15870-10-7

Physical Properties

Property code	Value	Unit	Source
af	0.3539		Cheméo Relay (1.0)
gf	95.77	kJ/mol	Joback Method
hf	-101.16	kJ/mol	Cheméo Relay (1.0)
hfus	13.89	kJ/mol	Joback Method
hvap	39.30	kJ/mol	NIST Webbook
ie	9.15	eV	Cheméo Relay (1.0)
log10ws	-4.37		Cheméo Relay (1.0)
logp	3.143		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
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	782.00		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
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rinpol	784.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	787.50		NIST Webbook
rinpol	784.30		NIST Webbook
rinpol	774.90		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	783.00		NIST Webbook
tb	393.15 ± 2.00	K	NIST Webbook
tb	393.15 ± 2.00	K	NIST Webbook
tb	392.50 ± 1.00	K	NIST Webbook
tb	392.65 ± 0.50	K	NIST Webbook
tb	392.45 ± 0.50	K	NIST Webbook
tb	391.65 ± 1.00	K	NIST Webbook
tb	392.75 ± 0.40	K	NIST Webbook
tb	392.45 ± 0.50	K	NIST Webbook
tb	392.37 ± 0.30	K	NIST Webbook
tb	392.00 ± 3.00	K	NIST Webbook
tb	391.65 ± 1.00	K	NIST Webbook
tb	389.65 ± 3.00	K	NIST Webbook
tb	392.50	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	183.01 ± 0.30	K	NIST Webbook
tf	183.05 ± 0.50	K	NIST Webbook
tf	183.01 ± 1.00	K	NIST Webbook
vc	0.453	m3/kmol	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15870107&Units=SI
Cheméo Relay (1.0):	
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol256.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
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